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PROGRAMS FOR CALCULATING RELATIVE INTENSITIES IN THE VIBRATIONAL STRUCTURE OF ELECTRONIC BAND SYSTEMS

Berkeley, California

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PROGRAMS FOR CALCULATING RELATIVE INTENSITIES IN THE VIBRATIONAL STRUCTURE OF ELECTRONIC BAND SYSTEMS*

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ABSTRACT

Source-deck listings of two computer programs are given for the calculation of relative intensities in the vibrational structure of an electronic transition. The first program finds turning points of an electronic potential-energy curve by direct numerical evaluation of the Klein action integrals in the RKR procedure. The second program uses these turning points to construct an effective potential for the molecule with rotational quantum number J. The radial Schrödinger equation then is solved for this potential to yield vibrational-rotational wavefunctions from which the program calculates Franck-Condon factors, r-centroids, and relative intensities.

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† Now at Harvard University, Cambridge, Massachusetts.

INTRODUCTION

This report supplements a previous paper,[1] hereafter referred to as I, which describes the calculation of relative intensities in the vibrational structure of an electronic transition. All computer programs used in I are documented herein.

Much of the programming was done by Mr. J. V. V. Kasper or in collaboration with him. The programs presented are not in final polished form and the author assumes the responsibility for all remaining errors that have gone undetected. No systematic attempt has been made to test all possible branches in these programs. However, these programs have been running successfully for over six months.

Much of the programming logic has been mentioned before in I. Comment cards have been liberally used in the Fortran source deck listings so that a description of the methods used in each program is self-contained. Comment cards also describe fully the preparation of data cards for each program. To further aid the user, sample data decks, which were successfully tested, are included. The output from these sample decks is displayed in the Appendix.

These programs are written for an IBM 709/7090/7094 installation. All source decks shown are photographic reproductions of machine listings.

PROGRAM FOR FINDING TURNING POINTS OF A POTENTIAL BY RKR PROCEDURE

Remarks

The input may be either in the form of spectroscopic constants for the electronic state, or the actual G(v) and B_v spectroscopic data. In the former case, the program requires about 3 sec per pair of turning points, whereas in the latter case[2] it is 5 sec. It is also possible to use a combination of input modes, i. e., vibrational constants and rotational B_v data, or vice versa.

When giving G(v) data, the zero-point energy may be assigned by the user, or found from extrapolation by the program. This latter feature allows the use of zero-line measurements or tabulated $\Delta G(v)$ data.

Limitations

(a) If tabulated G(v) or B_v data are used that have anomalous behavior, it is possible for the interpolation procedures NTRPSR or NTRPDP to fail.
(b) If less than eight G(v) or B_v data points are to be read in, NUST in subroutine RKR must be modified.
(c) Since errors tend to accumulate in the calculation of the turning points for each higher vibrational level, the potential curve is less accurate as the dissociation limit is approached.

Listing

Table I lists the source decks and Table II gives a sample data deck for the RKR program.

Table I. Source-deck listing for RKR program.

```
CMAIN FINDS TURNING POINTS FOR A MOLECULE BY RYDBERG-KLEIN-REES METHOD
C      ALL INPUT IS IN WAVE NUMBERS AND ANGSTROMS.
C      USER SPECIFIES CHOICE BETWEEN MASS UNITS BASED ON C12 = 12, OR
C      O16 = 16.
C      THE FOLLOWING COMMENT CARDS DESCRIBE THE PREPARATION OF DATA CARDS
C
      DIMENSION XI(200),YI(200),XO(3000),V(3000),S(3000),KV(200),
     Z          ETRIAL(200),QIRA(2),QIEN(3),QIMS(2),ZIMS(2),ZIRA(2),
     Z          ZIEN(3),ECALC(200),XPRN(5),VPRN(5),DTFRMT(10),
     Z          G(200),BV(200),FMT(24), U(200),RMIN(200),RMAX(200),
     Z          DUFMT(10),BVF(200)
      COMMON XI,YI,XO,V,XH,NSTA,N,MSTA,M,XMIN,XMAX,INSC,MBEG,NUSED,S,
     Z       NI,NS,MAXIT,FACM,ZMU,DE,WE,WEXE,WEYE,WEZE,WETE,BE,ALPHAE,
     Z       GAMMAE,DELTAE,AS,BS,MQ,STEP,U,BV,G,ICK,H,ITR,HDES,EPSLNE
C
C       FIRST CARD IN DATA HAS A ONE IN COLUMN 1 IF A PROBLEM FOLLOWS.
C       VERY LAST CARD IN DATA MUST BE A BLANK CARD.....
C
    1 CALL TIME(BEGIN)
      WRITEOUTPUTTAPE6,140,BEGIN
  140 FORMAT (9H0 TIME =   F10.5)
      READINPUTTAPE5,100,ITEST
  100 FORMAT (I1)
    2 IF (ITEST) 3,400,3
C
C       NEXT TWO CARDS IN DATA HAVE NAME OF PROBLEM IN COLUMNS 1-72,
C       WHERE CARRIAGE CONTROL IS IN COLUMN 1.  NEXT CARD HAS IIMS AND
C       MASSES OF THE TWO ATOMS, OR IIMS AND REDUCED MASS IN FIRST MASS
C       FIELD WITH SECOND BLANK.
C       IIMS = 1, MASS UNITS ARE BASED ON C12 = 12.
C       IIMS = 2, MASS UNITS ARE BASED ON O16 = 16.
C
    3 READINPUTTAPE5,101,(FMT(I),I=1,24)
  101 FORMAT (12A6)
      READINPUTTAPE5,102,IIMS,ZMAS1,ZMAS2
  102 FORMAT (I4,2F10.0)
C
C       NEXT CARD IN DATA HAS IQHK, AND NUMBER OF LEVELS, EACH
C       IN I4 FORMAT, AS WELL AS THE FORMAT STATEMENT WHICH CONTROLS THE
C       READING OF THE LEVELS (IN COLUMNS 13-72)--FOR EXAMPLE- (4E16.8).
C       IQHK = 0 IF THE FOLLOWING CARDS CONTAIN THE TABULATED G CURVE.
C       IF A PARTICULAR VALUE IS TO BE INTERPOLATED, SET G(I) = -10.
C       IF IT IS DESIRED TO USE CONSTANTS  TO GENERATE THE ENTIRE
C       G CURVE, IQHK MUST NOT BE EQUAL TO ZERO.
C       A HOLLERITH TEXT MUST BE PUNCHED IN COLUMNS 13-72,
C       AS IT WILL BE PRINTED, E.G.,    (1H )
C       THE NEXT CARD IN SUCH A CASE CONTAINS
C       WE,WEXE,WEYE,WEZE,AND WETE.
C
    5 READINPUTTAPE5,103,IQHK,      N,(DTFRMT(I),I=1,10)
103   FORMAT(2I4,4X,10A6)
      IIEN = 2
    6 IF (IQHK) 8,7,8
    8 READINPUTTAPE5,114,WE,WEXE,WEYE,WEZE,WETE
  114 FORMAT (5E10.0)
      GO TO 9
    7 READINPUTTAPE5,DTFRMT,(G(I),I=1,N)
C
```

Table I. (Contd.)

```
C     THE ZERO POINT ENERGY MAY BE FOUND BY EXTRAPOLATION, OR IT MAY BE
C     FIXED BY THE USER FROM HIS TABULATED G(V) CURVE.
C     NEXT CARD CONTAINS IOPEV.
C     SET IOPEV = 0, IF THE ZERO POINT ENERGY IS TO BE FOUND BY
C     EXTRAPOLATION, AND THE G(V) CURVE IS TO BE RAISED OR LOWERED
C     ACCORDINGLY.
C     THIS IS PARTICULARLY USEFUL IF DELTA G(V) DATA IS TO BE USED.
C     SET IOPEV = 1, IF THE TABULATED G(V) CURVE IS TO BE USED UNCHANGED
C     SET IOPEV = 2, IF THE G(V) CURVE IS TO BE CONSTRUCTED FROM CONSTAN
C
9     READ INPUT TAPE 5, 100, IOPEV
C
C      THE NEXT SET OF CARDS CONTAINS THE BV CURVE WITH THE SAME
C      RESTRICTIONS AS FOR G CURVE ABOVE.  NUMBER OF VALUES HERE MUST BE
C      EQUAL TO THE NUMBER ABOVE
C
      READINPUTTAPE5,103,IBHK,      N,(DUFMT(I),I=1,10)
      IIEB = 2
   30 IF (IBHK) 31,32,31
   31 READINPUTTAPE5,114,BE,ALPHAE,GAMMAE,DELTAE,EPSLNE
      GO TO 33
   32 READINPUTTAPE5,DUFMT,(BV(I),I=1,N)
C
C     THE ROTATIONAL CONSTANT BE MAY BE FOUND BY EXTRAPOLATION, OR IT
C     MAY BE FIXED BY THE USER.
C     NEXT CARD CONTAINS IOPA AND BEQUIL.
C     SET IOPA = 0, IF THE VALUE OF BE IS TO BE FOUND BY EXTRAPOLATION
C     FROM THE BV DATA READ IN.    LEAVE BEQUIL BLANK.
C     SET IOPA = 1, IF THE VALUE OF BE IS TO BE GIVEN BY BEQUIL.
C     SET IOPA = 2, IF ROTATIONAL CONSTANTS ARE USED.    LEAVE BEQUIL
C     BLANK.
C
33    READ INPUT TAPE 5,102,IOPA,BEQUIL
C
C     NEXT DATA CARD CONTAINS RE, THE INTERNUCLEAR EQUILIBRIUM DISTANCE.
C
      READ INPUT TAPE 5,106,RE
106   FORMAT(F10.0)
C
C     NEXT DATA CARD CONTAINS VSTART,VFIN,AND HDED WHEPE
C     TURNING POINTS ARE CALCULATED FROM VIBRATIONAL LEVEL VSTART TO
C     VFIN IN STEPS OF HDED      E.G. FROM 0.5 TO 20.5 IN STEPS OF 1.0.
C
      READ INPUT TAPE 5,114,VSTART,VFIN,HDED
C
C     NEXT CARD CONTAINS IOPFG.
C     SET IOPFG = 1, IF INTERMEDIATE STEPS IN THE EVALUATION OF THE
C     KLEIN ACTION INTEGRALS ARE TO BE PRINTED.
C     SET IOPFG = 0, IF INTERMEDIATE PRINT-OUT IS TO BE SKIPPED.
C     NORMALLY THE USER SHOULD SET IOPFG = 0.
C
      READ INPUT TAPE 5,100,IOPFG
C     THIS TERMINATES COMMENT CARDS ON THE PREPARATION OF DATA.
C     IF NO FURTHER PROBLEMS FOLLOW, REMEMBER TO ADD A BLANK CARD TO
C     THE DATA DECK.
C
C
      QIRA(2) = 6HANGST.
```

Table I. (Contd.)

```
      QIEN(2) = 6H1/CM                                                  MAIN 116
      QIMS(1) = 6HC12=12                                                MAIN 117
      QIMS(2) = 6HO16=16                                                MAIN 118
C                                                                       MAIN 119
C      PRINT HEADING                                                    MAIN 120
C                                                                       MAIN 121
      WRITEOUTPUTTAPE6,101,(FMT(I),I=1,24)                              MAIN 122
C                                                                       MAIN 123
C      PRINT THE MASSES AND THEIR UNITS.                                MAIN 124
C                                                                       MAIN 125
   10 IF (ZMAS2) 12,12,11                                               MAIN 126
   11 WRITEOUTPUTTAPE6,121,QIMS(IIMS),ZMAS1,ZMAS2                       MAIN 127
  121 FORMAT (///40H  THE MASSES OF THE TWO ATOMS, BASED ON A6, 6H, ARE MAIN 128
     Z        F10.6, 5H AND  F10.6///)                                  MAIN 129
      GO TO 20                                                          MAIN 130
   12 WRITEOUTPUTTAPE6,111,QIMS(IIMS),ZMAS1                             MAIN 131
  111 FORMAT (///46H  THE REDUCED MASS OF THE TWO ATOMS, BASED ON A6,   MAIN 132
     Z          5H, IS  F10.6///)                                       MAIN 133
C                                                                       MAIN 134
C                                                                       MAIN 135
C                                                                       MAIN 136
C      PRINT G(V) DATA, OR VIBRATIONAL CONSTANTS                        MAIN 137
C                                                                       MAIN 138
   20 IF (IQHK) 22,21,22                                                MAIN 139
   22 WRITEOUTPUTTAPE6,DTFRMT                                           MAIN 140
      WRITEOUTPUTTAPE6,116,WE,WEXE,WEYE,WEZE,WETE                       MAIN 141
  116 FORMAT (63H0 THE G(V) CURVE IS CONSTRUCTED FROM THE FOLLOWING INPUMAIN 142
     ZT DATA.  // 7H  WE = F10.3,8H, WEXE =F10.4,8H, WEYE =E10.5,8H, WEZMAIN 143
     ZE =E10.5,8H, WETE =E10.5 )                                        MAIN 144
      GO TO 40                                                          MAIN 145
   21 WRITEOUTPUTTAPE6,122,QIEN(IIEN)                                   MAIN 146
  122 FORMAT (32H  THE INPUT G VALUES, ENERGY IN A6,                    MAIN 147
     Z       18H, ARE GIVEN BELOW.  //)                                 MAIN 148
      WRITEOUTPUTTAPE6,115,(G(I),I=1,N)                                 MAIN 149
  115 FORMAT (1X10F11.3)                                                MAIN 150
      WRITEOUTPUTTAPE6,128                                              MAIN 151
  128 FORMAT (20X48HVALUES OF -10. ARE TO BE FOUND BY INTERPOLATION.)   MAIN 152
C                                                                       MAIN 153
C      PRINT BV DATA, OR ROTATIONAL CONSTANTS                           MAIN 154
C                                                                       MAIN 155
   40 IF (IBHK) 41,42,41                                                MAIN 156
   41 WRITEOUTPUTTAPE6,DUFMT                                            MAIN 157
      WRITEOUTPUTTAPE6,120,BE,ALPHAE,GAMMAE,DELTAE,EPSLNE               MAIN 158
  120 FORMAT (64H0 THE BV(V) CURVE IS CONSTRUCTED FROM THE FOLLOWING INPMAIN 159
     ZUT DATA. //7H  BE = 1PE11.5,10H, ALPHAE = E11.4,10H, GAMMAE =     MAIN 160
     Z E11.4,10H, DELTAE = E11.4, 10H, EPSLNE =  E11.4)                 MAIN 161
      GO TO 43                                                          MAIN 162
   42 WRITEOUTPUTTAPE6,127,QIEN(IIEB)                                   MAIN 163
  127 FORMAT (33H  THE INPUT BV VALUES, ENERGY IN A6,                   MAIN 164
     Z  18H, ARE GIVEN BELOW.  //)                                      MAIN 165
      WRITEOUTPUTTAPE6,129,(BV(I),I=1,N)                                MAIN 166
  129 FORMAT (1X10F11.6)                                                MAIN 167
      WRITEOUTPUTTAPE6,128                                              MAIN 168
C                                                                       MAIN 169
C      PRINT HEADING                                                    MAIN 170
43    WRITEOUTPUTTAPE6,101,(FMT(I),I=1,24)                              MAIN 171
C                                                                       MAIN 172
  200 IF (ZMAS2) 201,201,202                                            MAIN 173
```

Table I. (Contd.)

```
  201 ZMU = ZMAS1
      GO TO 204
  202 ZMU = ZMAS1*ZMAS2/(ZMAS1+ZMAS2)
  204 ZIMS(1) = 1.0
      ZIMS(2) = .9996784
      ZIRA(1) = 1.0
      ZIRA(2) = 1.889766
      ZMU = ZMU * ZIMS(IIMS)
      ZIEN(1) = ZMU * 3.643668E3
      ZIEN(2) = ZMU * 1.6610826E-2
      ZIEN(3) = ZMU * 1.339776E2
      FACM = 60.201702/ZMU
  206 XI(1) = 0.5
  207 DO 208 I = 2,N
      IL = I - 1
      XI(I) = XI(IL) + 1.0
  208 CONTINUE
      ZERO = 0.0
      WRITEOUTPUTTAPE7,101,(FMT(I),I=1,24)
      WRITEOUTPUTTAPE7,138,RE,ZERO
  138 FORMAT (1XF9.7,F10.3)
210   CALL RKR(RMIN,RMAX,VSTART,VFIN,HDED,NFIN,EV1,U,IQHK,IBHK,IOPEV,
     Z        IOPA,BEQUIL,IOPFG)
      GO TO 1
  400 CALL EXIT
      END
```

```
CRKR   FINDS TURNING POINTS FROM G(V) AND BV DATA, OR FROM CONSTANTS
       SUBROUTINE RKR(RMIN,RMAX,VSTA,VFIN,HDED,M,EV1,U,IQHK,IBHK,IOPEV,
     Z                IOPA,BEQUIL,IOPFG)
       DIMENSION                UEV(3000),EV(3000),BV(200),BI(3000),
     Z           TEMP(200),U(200),RMIN(200),RMAX(200),Y(200),Z(200),
     Z           ZOC(9),MZ(5),IZ(5),IB(40),IG(40)
D      DIMENSION V(200),G(200),BO(200),OEV(200),OV(200),XG(20),YG(20),
     Z           ZG(20),EPSH(1),AGAUS(5,20),XGAUS(5,20),VSTA(1),VFIN(1),
     Z           HDED(1),DENQ(20)
       COMMON Y,TEMP,UEV,EV,Q,NST,N,MST,M,XMIN,XMAX,INSC,MBEG,NUSED,BI,
     Z        NI,NS,MAXIT,FACM,ZMU,DE,WE,WEXE,WEYE,WEZE,WETE,BE,ALPHAE,
     Z        GAMMAE,DELTAE,   VNIN,BQ,MQ,SPEP,   U,BV,Z,ICK,H,  K,HDES
     Z        ,EPSLNE
       GFUNCF(X)= ((((((((WETE*X)+WEZE)*X)+WEYE)*X)-WEXE)*X)+WE)*X
       BFUNCF(X) = ((((((EPSLNE*X)+DELTAE)*X)+GAMMAE)*X)-ALPHAE)*X)+BE
C       FAC = (HPLANCK*NAV/8*PI**2*C)**.5*E8/ZMU**.5
       FAC = 4.1057859/SQRTF(ZMU)
       NPROB = 1
       NUST = 8
       EV1 = 0.0
  201  CALL TIME(BEGIN)
C
C       TURNING POINTS FOUND FOR V = VSTA,VFIN,HDED.
C
C      INTERPOLATE G(V) AND BV DATA
C
  202  JJ = 0
       JK = 0
       IJ = 0
       IK = 0
       HDES = .01
       MBEG = 1
       IF(IOPEV-1)3000,3001,3000
3001   EV1 = Z(1)
3000   WRITEOUTPUTTAPE6,114,NUST
  114  FORMAT (20H0 NUSED IN BESRKR = I2,1H.)
       DO 187 I = 1,N
       IF (Z(I) + 10.) 182,183,182
  182  IJ = IJ + 1
       TEMP(IJ) = Y(I)
       U(IJ) = Z(I)
       GO TO 184
  183  JJ = JJ + 1
       UEV(JJ) = Y(I)
       IG(JJ) = I
  184  IF (BV(I) + 10.) 185,186,185
  185  IK = IK + 1
       RMIN(IK) = Y(I)
       RMAX(IK) = BV(I)
       GO TO 187
  186  JK = JK + 1
       EV(JK) = Y(I)
       IB(JK) = I
  187  CONTINUE
       IF (JJ) 191,191,188
  188  CALL NTRPSR (TEMP,U,UEV,BI,HDES,IJ,JJ,VNIN,VN,INSC,MBEG,NUST)
       LOC = 8
       IF (INSC) 288,189,288
```

Table I. (Contd.)

```
  189 DO 190 I = 1,JJ
      IJ = IG(I)
      Z(IJ) = BI(I)
  190 CONTINUE
  191 IF (JK) 196,196,192
  192 CALL NTRPSR (RMIN,RMAX,EV,BI,HDES,IK,JK,VNIN,VN,INSC,MBEG,NUST)
      LOC = 9
  193 IF (INSC) 288,194,288
  194 DO 195 I = 1,JK
      IK = IB(I)
      BV(IK) = BI(I)
  195 CONTINUE
  196 IF (IQHK) 204,203,204
  204 EV1 = -GFUNCF(0.5)
      IOPEV = 0
      DO 170 I = 1,N
      Z(I) = GFUNCF(Y(I)) + EV1
  170 CONTINUE
      GO TO 211
  203 INTG = INTQ
      MBEG = 1
      M = 1
      UEV(1) = 0.
      HDES = 1.
      EV1 = -EV1
      IF (EV1) 211,206,206
  206 CALL NTRPSR(Y,Z,UEV,EV,HDES,N,M,VNIN,VN,INSC,MBEG,NUST)
      LOC = 1
  208 IF (INSC) 288,210,288
  210 EV1 = EV(1)
C     EV1 NOW CONTAINS THE ZERO POINT ENERGY BY EXTRAPOLATION.
  211 IF (IBHK) 171,207,171
  171 EV(1) = BE
      DO 172 I = 1,N
      BV(I) = BFUNCF(Y(I))
  172 CONTINUE
      GO TO 205
  207 IF (IOPA) 2071,2072,2071
 2071 EV(1) = BEQUIL
      GO TO 205
 2072 CALL NTRPSR (Y,BV,UEV,EV,HDES,N,M,VNIN,VN,INSC,MBEG,NUST)
C     EV(1) NOW CONTAINS BE BY EXTRAPOLATION
      LOC = 7
      IF (INSC) 288,205,288
  205 V(1) = 0.
      G(1) = 0.
      BO(1) = EV(1)
      DO 209 I = 1,N
      V(I+1) = Y(I)
      G(I+1) = Z(I)
      BO(I+1) = BV(I)
  209 CONTINUE
      NP = N + 1
      IF (IOPEV) 2091,2092,2091
 2091 CONTINUE
      EV1 = EV1 + G(2)
 2092 DO 213 I = 2,NP
      G(I) = G(I) - EV1
```

Table I. (Contd.)

```
      Y(I) = V(I)
      Z(I) = G(I)
      BV(I) = BO(I)
  213 CONTINUE
      IF (IOPEV) 2131,2132,2131
 2131 EV1 = -G(2)
 2132 IF (NPROB-17) 2133,2134,2133
 2134 M = 1
      EV(1) = DE
      CALL NTRPSR (Z,Y,EV,UEV,HDES,NP,M,VNIN,VN,INSC,MBEG,NUST)
      LOC = 2
      IF (INSC) 288,2135,288
 2135 NP = NP + 1
      Y(NP) = UEV
      V(NP) = UEV
      Z(NP) = DE
      G(NP) = DE
      BO(NP) = 0.
      BV(NP) = 0.
 2133 Y(1) = 0.
      Z(1) = 0.
      BV(1) = BO(1)
      VMIN = VSTA
      VN = VFIN
      HDES = HDED
      M = 0
      WRITEOUTPUTTAPE6,113,(Y(I),Z(I),I=1,NP)
  113 FORMAT (33H0 THE G(V) VALUES USED BELOW ARE / 6(4X1HV10X1HG4X) //
     Z        6(1XF7.3,F12.4))
      WRITEOUTPUTTAPE6,108,(Y(I),BV(I),I=1,NP)
  108 FORMAT (33H0 THE BV(V) VALUES USED BELOW ARE / 6(4X1HV9X2HBV4X) //
     Z        6(1XF7.3,F12.7))
      IF (IQHK) 215,212,215
  215 M = XFIXF((VFIN-VSTA)/HDED) + 1
      DO 217 I = 1,M
      OEV(I) = VSTA + FLOATF(I-1)*HDED
      OV(I) = GFUNCF(OEV(I))
  217 CONTINUE
      INSC = 0
      GO TO 218
  212 CALL NTRPDP(V,G,OEV,OV,HDED,NP,M,VSTA,VFIN,INSC,MBEG,NUST)
      LOC = 2
      WRITEOUTPUTTAPE6,106,HDES,VMIN,VN,MBEG,NUST,INSC,NP,M
  106 FORMAT (6H0HDES=1PE15.7,7H, VMIN=E15.7,5H, VN=E15.7,7H, MBEG=I5/
     Z9X7H, NUST=I5,7H, INSC=I5,4H, N=I5,4H, M=I5)
  218 WRITEOUTPUTTAPE6,109
  109 FORMAT (54H0 OUTPUT V,G--LEVELS AT WHICH TURNING POINTS ARE FOUND/
     Z        6(4X1HV10X1HG4X) //)
      WRITEOUTPUTTAPE6,107,(OEV(I),OV(I),I=1,M)
  107 FORMAT (6(1XF7.3,F12.4))
  214 IF (INSC) 288,216,288
  216 DO 219 I = 1,M
      TEMP(I) = OEV(I)
      U(I) = OV(I)
  219 CONTINUE
C
C     INTEGRATION CONSTANTS
C
```

Table I. (Contd.)

```
        STEP = .9
        MZ(1) = 101
        MZ(2) = 81
        MZ(3) = 61
        IZ(1) = 8
D       XGAUS(1,1) = .019855071751232
D       XGAUS(1,2) = .101666761293186
D       XGAUS(1,3) = .237233795041836
D       XGAUS(1,4) = .408282678752175
D       XGAUS(1,5) = 1. - XGAUS(1,4)
D       XGAUS(1,6) = 1. - XGAUS(1,3)
D       XGAUS(1,7) = 1. - XGAUS(1,2)
D       XGAUS(1,8) = 1. - XGAUS(1,1)
D       AGAUS(1,1) = .050614268145188
D       AGAUS(1,2) = .111190517226687
D       AGAUS(1,3) = .156853322938944
D       AGAUS(1,4) = .181341891689181
D       AGAUS(1,5) = AGAUS(1,4)
D       AGAUS(1,6) = AGAUS(1,3)
D       AGAUS(1,7) = AGAUS(1,2)
D       AGAUS(1,8) = AGAUS(1,1)
        IZ(2) = 6
D       XGAUS(2,1) = .033765242898424
D       XGAUS(2,2) = .169395306766868
D       XGAUS(2,3) = .380690406958402
D       XGAUS(2,4) = 1. - XGAUS(2,3)
D       XGAUS(2,5) = 1. - XGAUS(2,2)
D       XGAUS(2,6) = 1. - XGAUS(2,1)
D       AGAUS(2,1) = .085662246189585
D       AGAUS(2,2) = .180380786524070
D       AGAUS(2,3) = .233956967286345
D       AGAUS(2,4) = AGAUS(2,3)
D       AGAUS(2,5) = AGAUS(2,2)
D       AGAUS(2,6) = AGAUS(2,1)
        IZ(3) = 4
D       XGAUS(3,1) = .069431844202974
D       XGAUS(3,2) = .330009478207572
D       XGAUS(3,3) = 1. - XGAUS(3,2)
D       XGAUS(3,4) = 1. - XGAUS(3,1)
D       AGAUS(3,1) = .173927422568727
D       AGAUS(3,2) = .326072577431273
D       AGAUS(3,3) = AGAUS(3,2)
D       AGAUS(3,4) = AGAUS(3,1)
D       ZG(1) = ZG(3)
        WRITEOUTPUTTAPE6,100
    100 FORMAT (1H1)
    224 DO 280 I = 1,M
D       TEMPI = OEV(I)
        NUS2 = NUST/2
        NB = NUS2 + 1
        NF = N - NB + 1
        DO 225 J = NB,NF
        IF (TEMPI - V(J)) 235,235,225
    225 CONTINUE
        ISG = NF + 1
        GO TO 237
    235 ISG = J
    237 NSTA = ISG - NUS2
```

Table I. (Contd.)

```
D       VMIN = 0.
        FEG = 0.
        GEG = 0.
        LT = 1
        IZGD = 0
        GDO = 0.
        FDO = 0.
        ISG = 0
        ISB = 0
C
C       COMMENCE FINDING TURNING POINTS BY INTEGRATION
C
        CALL TIME (BEGIA)
D   226 BS = VMIN + (TEMPI - VMIN) * STEP
    227 IF (LT-3) 228,228,301
    228 MQ = MZ(LT)
    223 KM = (MQ-1)/2
        TMIN = VMIN
        TS = BS
        A = (TS-TMIN)/FLOATF(MQ-1)
        MX = 0
        IF (IQHK) 401,229,401
    229 CALL NTRPSR(Y,Z,UEV,EV,A,NP,MX,TMIN,TS,INSC,MBEG,NUST)
    230 LOC = 3
    231 IF (INSC) 288,232,288
    232 IF (GDO) 236,233,236
    233 MX = 0
        IF (IBHK) 403,239,403
    239 CALL NTRPSR(Y,BV,UEV,BI,A,NP,MX,TMIN,TS,INSC,MBEG,NUST)
        LOC = 4
    234 IF (INSC) 288,236,288
    236 DO 238 J = 1,MQ
        DENQ = U(I) - EV(J)
        IF (DENQ) 292,292,241
    241 UEV(J) = 1./SQRTF(DENQ)
        EV(J) = BI(J) * UEV(J)
    238 CONTINUE
        FSUM = UEV(1) + 4.*UEV(2) + UEV(MQ)
        GSUM = EV(1) + 4.*EV(2) + EV(MQ)
    240 DO 242 J = 2,KM
        FSUM = FSUM + 4.*UEV(2*J) + 2.*UEV(2*J-1)
        GSUM = GSUM + 4.*EV(2*J) + 2.*EV(2*J-1)
    242 CONTINUE
        FEG2 = A*FSUM/3.
        GEG2 = A*GSUM/3.
    250 IF (LT - 1) 262,262,254
    301 IZDO = (LT-1)/3
        IF (IZDO - 3) 304,304,303
    303 IZDO = 3
    304 NGAS = IZ(IZDO)
        DO 306 J = 1,NGAS
D       XG(J) = (BS-VMIN) * XGAUS(IZDO,J) + VMIN
        UEV(J) = XG(J)
    306 CONTINUE
        MST = 1
D       EPSH = TEMPI - XG(NGAS)
        FEPS = EPSH
        IF (EPSH(1)) 276,307,308
```

Table I. (Contd.)

```
    307 IF (EPSH(2)) 276,276,308
    308 IF (IQHK) 405,309,405
    309 CALL NTRPDP(V,G,XG,YG,EPSH,NP,NGAS,VMIN,BS,INSC,MST,NUST)
        LOC = 5
    310 IF (INSC) 288,311,288
    311 IF (IZGD) 312,312,340
    312 IF (GDO)  318,314,318
    314 MST = 1
        IF (IBHK) 407,315,407
    315 CALL NTRPSR (Y,BV,UEV,BI,FEPS,NP,NGAS,TMIN,TS,INSC,MST,NUST)
        LOC = 6
    316 IF (INSC) 288,318,288
    318 FSUM = 0.0
        GSUM = 0.0
        DO 320 J = 1,NGAS
        IF (IQHK) 718,317,718
D   317 DENQ(J) = OV(I) - YG(J)
    718 IF (DENQ(J)) 292,292,323
    323 XG(J) = AGAUS(IZDO,J)/SQRTF(DENQ(J))
        YG(J) = BI(J) * XG(J)
        FSUM = FSUM + XG(J)
        GSUM = GSUM + YG(J)
    320 CONTINUE
        IF (BI(NGAS)-BI(1)) 322,321,322
    321 IZGD = 1
D   322 BSV = BS - VMIN
        FEG2 = BSV * FSUM
    324 GEG2 = BSV * GSUM
        GO TO 254
    340 FSUM = 0.0
        DO 342 J = 1,NGAS
D       DENQ = OV(I) - YG(J)
        IF (DENQ) 292,292,341
    341 XG(J) = AGAUS(IZDO,J)/SQRTF(DENQ)
        FSUM = FSUM + XG(J)
    342 CONTINUE
        GSUM = BI(NGAS) * FSUM
        GO TO 322
    254 IF (FEG2/FEG - 1.E-6) 255,255,256
    255 FDO = 1.
    256 IF (GEG2/GEG - 1.E-6) 257,257,258
    257 GDO = 1.
    258 IF (ABSF(FEG2/FEG1) - .9) 260,260,259
    259 FDO = 1.
    260 IF (ABSF(GEG2/GEG1) - .9) 262,262,261
    261 GDO = 1.
    262 LT = LT + 1
        FEG1 = FEG2
        GEG1 = GEG2
    264 IF (FDO) 269,266,269
    266 FEG = FEG + FEG2
    268 IF (GDO) 272,270,272
    269 IF (GDO) 276,270,276
    270 GEG = GEG + GEG2
D   272 VMIN = BS
        IF (IOPFG) 273,274,273
    273 CALL TIME (AFTEA)
        XTIQ = (AFTEA-BEGIA)*60.
```

Table I. (Contd.)

```
      BEGIA = AFTEA
      WRITEOUTPUTTAPE6,110,FEG,GEG,XTIQ
  110 FORMAT (6X6HFEG = 1PE15.7, 8H, GEG = E15.7,10X9HPEQUIRED 0PF8.5,
     Z         9H SECONDS.)
  274 IF (LT-20) 226,226,290
  276 F = FEG * FAC
      GF = GEG / FAC
      RMAX(I) = SQRTF(F*F + F/GF) + F
      RMIN(I) = RMAX(I) - 2.*F
      CALL TIME(AFTER)
      XTIQ = 60.*(AFTER-BEGIN)
      BEGIN = AFTER
      WRITEOUTPUTTAPE6,104,TEMPI,U(I),RMIN(I),RMAX(I),XTIQ,BI(NGAS)
     Z                     ,F,GF
  104 FORMAT (10H0 FOR V = F7.3,6H, G = F10.3,14H 1/CM, RMIN = F10.7,
     Z         12H AND RMAX = F10.7,27H ANGSTROMS.  THIS REQUIRED F8.5,
     Z         9H SECONDS. / 20X12H ALSO, BV =  F12.7 /20X49H THE KLEIN A
     ZCTION INTEGRALS F AND G ARE EQUAL TO   2E15.8///)
      WRITEOUTPUTTAPE7,105,RMIN(I),U(I),RMAX(I),U(I)
  105 FORMAT (1XF9.7,F10.3 / 1XF9.7,F10.3)
  280 CONTINUE
      DO 284 I = 1,N
      Z(I) = Z(I+1)
      Y(I) = Y(I+1)
      BV(I) = BV(I+1)
  284 CONTINUE
      WRITEOUTPUTTAPE6,100
  286 RETURN
  288 ZOC(1) = 6H EV1
      ZOC(2) = 6HG(LEV)
      ZOC(3) = 6HS.P.EV
      ZOC(4) = 6HS.P.BV
      ZOC(5) = 6HD.P.EV
      ZOC(6) = 6HD.P.BV
      ZOC(7) = 6H BV1
      ZOC(8) = 6HG FILL
      ZOC(9) = 6HBVFILL
      WRITEOUTPUTTAPE6,102,ZOC(LOC),U(I)
  102 FORMAT (26H0 NTRPDP UNSUCCESSFUL FOR A6, 11H, WHEN U =  E16.8)
      INTG = 1
      GO TO 286
  290 WRITEOUTPUTTAPE6,103
  103 FORMAT (20H0 TEG REACHED MAXIT   )
      INTG = 1
      GO TO 286
  292 INTG = 1
      WRITEOUTPUTTAPE6,111
  111 FORMAT (22H0 DENQ IS NOT POSITIVE)
      GO TO 286
  401 MX = MQ
      DO 402 J = 1,MQ
      UEV(J) = TMIN + FLOATF(J-1) * A
      EV(J) = GFUNCF(UEV(J))
  402 CONTINUE
      GO TO 232
  403 MX = MQ
      DO 404 J = 1,MQ
      UEV(J) = TMIN + FLOATF(J-1) * A
```

Table I. (Contd.)

```
      BI(J) = BFUNCF(UEV(J))
  404 CONTINUE
      GO TO 236
  405 CALL DGUNC (XG,DENQ,NGAS,TEMPI)
      GO TO 311
  407 DO 408 J = 1,NGAS
      BI(J) = BFUNCF(UEV(J))
  408 CONTINUE
      GO TO 318
      END
```

Table I. (Contd.) UCRL-10925

```
CNTRPSR  INTERPOLATION PROGRAM (BY SUCCESSIVE RANGES)  SINGLE PREC.
C
C      THE METHOD OF LAGRANGE IS USED.  THE INPUT POINTS NEED NOT BE
C      EQUALLY SPACED.  THERE ARE TWO MODES OF INPUT AVAILABLE.  THE
C      FIRST OCCURS WHEN M = 0.  THE ABSCISSAE ARE THEN GENERATED FROM
C      XMIN,XMAX,AND XH.  AT EXIT M = NO. OF POINTS FOUND, AND XO
C      CONTAINS THE ABSCISSAE.  M WILL BE CHECKED TO INSURE THAT THE
C      DIMENSION IS NOT EXCEEDED.  MDIMM = THE DIMENSION OF THE XO, YO
C      ARRAYS.  THE SECOND MODE OCCURS WHEN M IS POSITIVE.  THE M
C      ABSCISSAE ARE THEN ASSUMED TO HAVE BEEN GENERATED PRIOR TO
C      ENTRY.  THE STARTING INDEX FOR THE OUTPUT ARRAY MUST BE
C      SPECIFIED.  THE FIRST POINT FOUND WILL BE AT XO(MBEG).  XH MUST
C      BE GIVEN SINCE THE ORDINATE FOR ANY POINT CLOSER THAN .01*XH TO
C      AN INPUT POINT IS TAKEN AS THAT FOR THE INPUT POINT.  -NUSED- IS
C      THE NUMBER OF POINTS USED FOR EACH INTERPOLATED POINT.  *NUSED*
C      MUST BE EVEN AND LESS THAN OR EQUAL TO -N-.  NUSED = 8 IS
C      SUGGESTED.  ANY POINT FARTHER THAN NUSED/2 POINTS FROM EITHER END
C      IS FOUND FROM THE NUSED/2 ON EACH SIDE.  NTRPSR WILL SCALE AND
C      RESCALE IN ORDER TO AVOID OVERFLOW.  IF THE FIRST SCALING DOES
C      NOT SUCCEED, NTRPSR WILL TRY UP TO 7 TIMES MORE BEFORE RETURNING
C      IN THE ERROR MODE. (INSC = 1)
C      INPUT IS  XI,YI,(XO),XH,N,M,(XMIN),(XMAX),MBEG,NUSED.
C      OUTPUT IS  (XO),YO,INSC.
C      INSC = 0 IF PROGRAM WAS SUCCESSFUL.  IF NOT, INSC = 1.
C
      SUBROUTINE NTRPSR(XJ,YJ,XO,YO,XN,N,K,XNIN,XNAX,INSC,MBEG,NUSED)
      DIMENSION XI(200),YI(200),XO(3000),YO(3000),XJ(200),YJ(200),
     Z          NUMB(200)
      MDIMM = 3000
      XMAX = XNAX
      XMIN = XNIN
      XH = ABSF(XN)
      M = K
      IREV = 0
      IREX = 0
C     M IS ZERO, IF XH, XMIN, XMAX ARE TO BE USED.  IF M IS NOT = TO
C     ZERO, THEN XO(I), I = 1,M WILL BE USED AS ABSCISSA.
  200 IF (M) 270,201,206
  201 M = XINTF(ABSF((XMAX-XMIN)/XH)) + 1
C     IF M IS MORE THAN DIMENSION OF XO, RETURN IN ERROR MODE.
      IF (M+MBEG-MDIMM-2) 202,272,272
  202 MF = MBEG + M - 1
      IF (XMAX - XMIN) 203,204,204
  203 XMIN = XNAX
      XMAX = XNIN
      IREV = 1
  204 DO 205 I = MBEG,MF
      XO(I) = FLOATF(I-MBEG) * XH + XMIN
  205 CONTINUE
  206 DO 207 I = 1,N
      XI(I) = XJ(I)
  207 CONTINUE
      MF = MBEG + M - 1
      MSTA = MBEG
      NUST = NUSED/2
      NS = NUST + 1
      NF = N - NS + 1
      NFP = NF + 1
```

Table I. (Contd.)

```
      DO 208 I = NS,NFP                                      NTRPS058
      NUMB(I) = 0                                            NTRPS059
  208 CONTINUE                                               NTRPS060
      IF (XO(MF) - XO(MBEG)) 209,211,211                     NTRPS061
  209 M2 = M/2                                               NTRPS062
      M2F = MBEG + M2 - 1                                    NTRPS063
      DO 210 I = MBEG,M2F                                    NTRPS064
      K = MF + MBEG - I                                      NTRPS065
      TEMP = XO(I)                                           NTRPS066
      XO(I) = XO(K)                                          NTRPS067
      XO(K) = TEMP                                           NTRPS068
  210 CONTINUE                                               NTRPS069
      IREV = 1                                               NTRPS070
  211 IF (XI(N)-XI(1)) 212,216,216                           NTRPS071
  212 N2 = N/2                                               NTRPS072
      DO 214 I = 1,N2                                        NTRPS073
      K = N + 1 - I                                          NTRPS074
      TEMP = XJ(I)                                           NTRPS075
      TEMS = YJ(I)                                           NTRPS076
      XJ(I) = XJ(K)                                          NTRPS077
      YJ(I) = YJ(K)                                          NTRPS078
      XJ(K) = TEMP                                           NTRPS079
      YJ(K) = TEMS                                           NTRPS080
  214 CONTINUE                                               NTRPS081
      IREX = 1                                               NTRPS082
  216 IF (NF-NS) 236,218,218                                 NTRPS083
  218 DO 226 J = MBEG,MF                                     NTRPS084
      DO 224 I = NS,NF                                       NTRPS085
  220 IF (XO(J) - XI(I)) 222,222,224                         NTRPS086
  222 NUMB(I) = NUMB(I) + 1                                  NTRPS087
      GO TO 226                                              NTRPS088
  224 CONTINUE                                               NTRPS089
      NUMB(NFP) = NUMB(NFP) + 1                              NTRPS090
  226 CONTINUE                                               NTRPS091
      GO TO 238                                              NTRPS092
  236 NUMB(NFP) = M                                          NTRPS093
  238 M = 0                                                  NTRPS094
  239 DO 250 L = NS,NFP                                      NTRPS095
      IF (NUMB(L)) 250,250,242                               NTRPS096
  242 M = NUMB(L)                                            NTRPS097
      NSTA = L - NUST                                        NTRPS098
      GO TO 100                                              NTRPS099
  246 IF (INSC) 274,248,274                                  NTRPS100
  248 MSTA = MSTA + M                                        NTRPS101
  250 CONTINUE                                               NTRPS102
  240 K = MSTA - MBEG                                        NTRPS103
      IF (IREV) 256,256,252                                  NTRPS104
  252 M2F = K/2 + MBEG - 1                                   NTRPS105
      DO 254 I = MBEG,M2F                                    NTRPS106
      J = MF + MBEG - I                                      NTRPS107
      TEMP = XO(I)                                           NTRPS108
      TEMS = YO(I)                                           NTRPS109
      XO(I) = XO(J)                                          NTRPS110
      YO(I) = YO(J)                                          NTRPS111
      XO(J) = TEMP                                           NTRPS112
      YO(J) = TEMS                                           NTRPS113
  254 CONTINUE                                               NTRPS114
  256 IF (IREX) 262,262,258                                  NTRPS115
```

Table I. (Contd.)

```
  258 DO 260 I = 1,N2
      J = N + 1 - I
      TEMP = XJ(I)
      TEMS = YJ(I)
      XJ(I) = XJ(J)
      YJ(I) = YJ(J)
      XJ(J) = TEMP
      YJ(J) = TEMS
  260 CONTINUE
  262 RETURN
  270 WRITEOUTPUTTAPE6,2101
 2101 FORMAT (44H0 ERROR IN INPUT TO NTRPSR.  M IS NEGATIVE.    )
      INSC = 1
      GO TO 240
  272 H = (XMAX-XMIN)/FLOATF(MDIMM-MBEG)
      WRITEOUTPUTTAPE6,2102,H
 2102 FORMAT (58H0 ERROR IN INPUT TO NTRPSR.  MINIMUM ALLOWABLE SPACING
     8IS      1PE12.3)
      INSC = 1
      GO TO 240
  274 WRITEOUTPUTTAPE6,2103,L
 2103 FORMAT (43H0 INTR1 WAS UNABLE TO INTERPOLATE IN RANGE     I3)
      GO TO 240
  100 NCON = 1
      REFA = 1.414214
      NFIN = NSTA + NUSED - 1
      DO 98 I = NSTA,NFIN
      XI(I) = XJ(I)
      YI(I) = YJ(I)
   98 CONTINUE
      NSTA1 = NSTA + 1
      XSCALE = (XI(NFIN) - XI(NSTA))/10.
      YMAX = YI(NSTA)
      YMIN = YI(NSTA)
 1001 DO 1002 I = NSTA1,NFIN
      YMAX = MAX1F(YMAX,YI(I))
      YMIN = MIN1F(YMIN,YI(I))
 1002 CONTINUE
   91 YSCALE = YMAX - YMIN
 1003 DO 1004 I = NSTA,NFIN
      XI(I) = XI(I)/XSCALE
      YI(I) = (YI(I)-YMIN)/YSCALE + .5
 1004 CONTINUE
      XH = ABSF(XN)/XSCALE
      MFIN = MSTA + M - 1
      MTA = MSTA
 1005 EPSIL = .01*XH
  101 DO 110 II=  MTA,MFIN
      XO(II) = XO(II)/XSCALE
      YO(II) = 0.0
      PNUM = 1.0
 1011 DO 107 I = NSTA,NFIN
C     FIND XO(II)-XI(I) FOR NUMERATOR AND CHECK FOR NEARNESS.
      XNUM     = XO(II) - XI(I)
 1012 IF (ABSF(XNUM    )-EPSIL) 102,102,103
  102 YO(II) = YI(I)
      GO TO 109
C     PNUM = PRODUCT OF ALL XNUM
```

Table I. (Contd.)

```
  103 PNUM = PNUM*XNUM
C     CONSTRUCT DENOMINATOR AND SUM
      PDEN = 1.0
  104 DO 106 J = NSTA,NFIN
 1043 IF (I-J) 105,106,105
  105 PDEN =       (XI(I) - XI(J))*PDEN
 1051 IF QUOTIENT OVERFLOW 1103,106
  106 CONTINUE
      DEN = PDEN*XNUM
      YO(II) = YI(I)/DEN + YO(II)
      IF ACCUMULATOR OVERFLOW  1121, 107
  107 CONTINUE
      YO(II) = YO(II)*PNUM
  109 YO(II) = (YO(II)-.5)*YSCALE + YMIN
      XO(II) = XO(II) * XSCALE
  110 CONTINUE
      INSC = 0
      GO TO 246
 1103 WRITEOUTPUTTAPE6,1104,NCON,XSCALE
      WRITEOUTPUTTAPE6,1108,II,I,J
 1104 FORMAT (8H  NCON = I3, 11H, XSCALE =   F10.7)
 1108 FORMAT (26H  OVERFLOW OCCURRED AT II= I4,4H  I= I3,4H  J= I3)
      NCON = NCON + 1
 1105 DO 1106 I = NSTA,NFIN
      XI(I) = XI(I)/REFA
 1106 CONTINUE
      XO(II) = XO(II) * XSCALE
      MTA = II
      XH   = XH  /REFA
      XSCALE = XSCALE*REFA
      IF (NCON-8)  1005,1005,1107
 1107 INSC = 1
      GO TO 246
 1121 WRITEOUTPUTTAPE6,1122
 1122 FORMAT (48H0 ACCUMULATOR OVERFLOW.  DEN MUST BE TOO SMALL.    )
      INSC = 1
      GO TO 246
      FREQUENCY 1051(1,9),1001(50),1003(50),101(500),1011(50),
     1  1012(0,0,1),104(50),1043(1,0,1)
      END
```

Table I. (Contd.)

```
CNTRPDP  INTERPOLATION PROGRAM(BY SUCCESSIVE RANGES) DOUBLE PRECISION.
C
C        THE METHOD OF LAGRANGE IS USED.  THE INPUT POINTS NEED NOT BE
C        EQUALLY SPACED.  THERE ARE TWO MODES OF INPUT AVAILABLE.  THE
C        FIRST OCCURS WHEN M = 0.  THE ABSCISSAE ARE THEN GENERATED FROM
C        XMIN,XMAX,AND XH.  AT EXIT M = NO. OF POINTS FOUND, AND XO
C        CONTAINS THE ABSCISSAE.  M WILL BE CHECKED TO INSURE THAT THE
C        DIMENSION IS NOT EXCEEDED.  MDIMM = THE DIMENSION OF THE XO, YO
C        ARRAYS.  THE SECOND MODE OCCURS WHEN M IS POSITIVE.  THE M
C        ABSCISSAE ARE THEN ASSUMED TO HAVE BEEN GENERATED PRIOR TO
C        ENTRY.  THE STARTING INDEX FOR THE OUTPUT ARRAY MUST BE
C        SPECIFIED.  THE FIRST POINT FOUND WILL BE AT XO(MBEG).  XH MUST
C        BE GIVEN SINCE THE ORDINATE FOR ANY POINT CLOSER THAN .01*XH TO
C        AN INPUT POINT IS TAKEN AS THAT FOR THE INPUT POINT.  -NUSED- IS
C        THE NUMBER OF POINTS USED FOR EACH INTERPOLATED POINT.  *NUSED*
C        MUST BE EVEN AND LESS THAN OR EQUAL TO -N-.  NUSED = 8 IS
C        SUGGESTED.  ANY POINT FARTHER THAN NUSED/2 POINTS FROM EITHER END
C        IS FOUND FROM THE NUSED/2 ON EACH SIDE.  NTRPSR WILL SCALE AND
C        RESCALE IN ORDER TO AVOID OVERFLOW.  IF THE FIRST SCALING DOES
C        NOT SUCCEED, NTRPSR WILL TRY UP TO 7 TIMES MORE BEFORE RETURNING
C        IN THE ERROR MODE. (INSC = 1)
C        INPUT IS  XI,YI,(XO),XH,N,M,(XMIN),(XMAX),MBEG,NUSED.
C        OUTPUT IS  (XO),YO,INSC.
C        INSC = 0 IF PROGRAM WAS SUCCESSFUL.  IF NOT, INSC = 1.
C
      SUBROUTINE NTRPDP(XJ,YJ,XO,YO,XN,N,K,XNIN,XNAX,INSC,MBEG,NUSED)
D     DIMENSION XI(200),YI(200),XJ(200),YJ(200),XO(200),YO(200),XMIN(1),
     Z          XMAX(1),XNUM(1),EPSIL(1)
      DIMENSION NUMB(200)
      MDIMM = 200
D     XMAX = XNAX
D     XMIN = XNIN
D     XH   = XN
      M = K
C     M IS ZERO, IF XH IS TO BE USED.  IF NOT, XH=(XMAX-XMIN)/(M-1).
  200 IF (M) 270,201,205
D 201 M =  INTF((XMAX - XMIN)/XH) + 1.
C     IF M IS MORE THAN DIMENSION OF XO, RETURN IN ERROR MODE.
  202 IF (M+MBEG-MDIMM-2) 203,272,272
  203 MF = MBEG + M - 1
      DO 204 I = MBEG,MF
D     XO(I) = FLOATF(I-MBEG) * XH + XMIN
  204 CONTINUE
  205 DO 206 I = 1,N
D     XI(I) = XJ(I)
  206 CONTINUE
      MF = MBEG + M - 1
      MSTA = MBEG
      NUST = NUSED/2
      NS = NUST + 1
      NF = N - NS + 1
      NFP = NF + 1
      DO 207 I = NS,NFP
      NUMB(I) = 0
  207 CONTINUE
  209 IF (NF-NS) 236,210,210
  210 DO 226 J = MBEG,MF
      DO 224 I = NS,NF
```

Table I. (Contd.)

```
 214 IF (XO(J) - XI(I)) 216,215,224                                    NTRPD058
 215 IF (XO(J+20 )-XI(I+200)) 216,216,224                              NTRPD059
 216 NUMB(I) = NUMB(I) + 1                                             NTRPD060
     GO TO 226                                                         NTRPD061
 224 CONTINUE                                                          NTRPD062
     NUMB(NFP) = NUMB(NFP) + 1                                         NTRPD063
 226 CONTINUE                                                          NTRPD064
     GO TO 238                                                         NTRPD065
 236 NUMB(NFP) = M                                                     NTRPD066
 238 M = 0                                                             NTRPD067
 239 DO 250 L = NS,NFP                                                 NTRPD068
     IF (NUMB(L)) 250,250,242                                          NTRPD069
 242 M = NUMB(L)                                                       NTRPD070
     NSTA = L - NUST                                                   NTRPD071
     GO TO 100                                                         NTRPD072
 246 IF (INSC) 274,248,274                                             NTRPD073
 248 MSTA = MSTA + M                                                   NTRPD074
 250 CONTINUE                                                          NTRPD075
 240 K = MSTA - MBEG                                                   NTRPD076
     RETURN                                                            NTRPD077
 270 WRITEOUTPUTTAPE6,2101                                             NTRPD078
2101 FORMAT (44H0 ERROR IN INPUT TO NTRPSR.  M IS NEGATIVE.    )       NTRPD079
     INSC = 1                                                          NTRPD080
     GO TO 240                                                         NTRPD081
 272 H = (XMAX-XMIN)/FLOATF(MDIMM-MBEG)                                NTRPD082
     WRITEOUTPUTTAPE6,2102,H                                           NTRPD083
2102 FORMAT (58H0 ERROR IN INPUT TO NTRPSR.  MINIMUM ALLOWABLE SPACING NTRPD084
    8IS      1PE12.3)                                                  NTRPD085
     INSC = 1                                                          NTRPD086
     GO TO 240                                                         NTRPD087
 274 WRITEOUTPUTTAPE6,2103,L                                           NTRPD088
2103 FORMAT (43H0 INTR1 WAS UNABLE TO INTERPOLATE IN RANGE     I3)     NTRPD089
     GO TO 240                                                         NTRPD090
 100 NCON = 1                                                          NTRPD091
     REFA = 1.414214                                                   NTRPD092
     NFIN = NSTA + NUSED - 1                                           NTRPD093
     DO 98 I = NSTA,NFIN                                               NTRPD094
D    XI(I) = XJ(I)                                                     NTRPD095
D    YI(I) = YJ(I)                                                     NTRPD096
  98 CONTINUE                                                          NTRPD097
     NSTA1 = NSTA + 1                                                  NTRPD098
     XSCALE = (XI(NFIN) - XI(NSTA))/10.                                NTRPD099
     YMAX = YI(NSTA)                                                   NTRPD100
     YMIN = YI(NSTA)                                                   NTRPD101
1001 DO 1002 I = NSTA1,NFIN                                            NTRPD102
     YMAX = MAX1F(YMAX,YI(I))                                          NTRPD103
     YMIN = MIN1F(YMIN,YI(I))                                          NTRPD104
1002 CONTINUE                                                          NTRPD105
D 91 YSCALE = YMAX - YMIN                                              NTRPD106
1003 DO 1004 I = NSTA,NFIN                                             NTRPD107
D    XI(I) = XI(I)/XSCALE                                              NTRPD108
D    YI(I) = (YI(I)-YMIN)/YSCALE + .5                                  NTRPD109
1004 CONTINUE                                                          NTRPD110
D    XH   = XN  /XSCALE                                                NTRPD111
     MFIN = MSTA + M - 1                                               NTRPD112
     MTA = MSTA                                                        NTRPD113
D1005 EPSIL = .01*XH                                                   NTRPD114
 101 DO 110 II=  MTA,MFIN                                              NTRPD115
```

Table I. (Contd.)

```
D      XO(II) = XO(II)/XSCALE                                          NTRPD116
D      YO(II) = 0.0                                                    NTRPD117
D      PNUM = 1.0                                                      NTRPD118
 1011 DO 107 I = NSTA,NFIN                                             NTRPD119
C      FIND XO(II)-XI(I) FOR NUMERATOR AND CHECK FOR NEARNESS.         NTRPD120
D      XNUM    = XO(II) - XI(I)                                        NTRPD121
 1012 IF (ABSF(XNUM   )-EPSIL) 102,1013,103                            NTRPD122
 1013 IF (ABSF(XNUM(2))-EPSIL(2)) 102,102,103                          NTRPD123
D 102 YO(II) = YI(I)                                                   NTRPD124
      GO TO 109                                                        NTRPD125
C      PNUM = PRODUCT OF ALL XNUM                                      NTRPD126
D 103 PNUM = PNUM*XNUM                                                 NTRPD127
C      CONSTRUCT DENOMINATOR AND SUM                                   NTRPD128
D      PDEN = 1.0                                                      NTRPD129
  104 DO 106 J = NSTA,NFIN                                             NTRPD130
 1043 IF (I-J) 105,106,105                                             NTRPD131
D 105 PDEN =        (XI(I) - XI(J))*PDEN                               NTRPD132
 1051 IF QUOTIENT OVERFLOW 1103,106                                    NTRPD133
  106 CONTINUE                                                         NTRPD134
D      DEN = PDEN*XNUM                                                 NTRPD135
D      YO(II) = YI(I)/DEN + YO(II)                                     NTRPD136
      IF ACCUMULATOR OVERFLOW  1121, 107                               NTRPD137
  107 CONTINUE                                                         NTRPD138
D      YO(II) = YO(II)*PNUM                                            NTRPD139
D 109 YO(II) = (YO(II)-.5)*YSCALE + YMIN                               NTRPD140
D      XO(II) = XO(II) * XSCALE                                        NTRPD141
  110 CONTINUE                                                         NTRPD142
      INSC = 0                                                         NTRPD143
      GO TO 246                                                        NTRPD144
 1103 WRITEOUTPUTTAPE6,1104,NCON,XSCALE                                NTRPD145
      WRITEOUTPUTTAPE6,1108,II,I,J                                     NTRPD146
 1104 FORMAT (8H  NCON = I3, 11H, XSCALE =    F10.7)                   NTRPD147
 1108 FORMAT (26H  OVERFLOW OCCURRED AT II= I4,4H  I= I3,4H  J= I3)    NTRPD148
      NCON = NCON + 1                                                  NTRPD149
 1105 DO 1106 I = NSTA,NFIN                                            NTRPD150
D      XI(I) = XI(I)/REFA                                              NTRPD151
 1106 CONTINUE                                                         NTRPD152
D      XO(II) = XO(II) * XSCALE                                        NTRPD153
      MTA = II                                                         NTRPD154
D      XH   = XH  /REFA                                                NTRPD155
D      XSCALE = XSCALE*REFA                                            NTRPD156
      IF (NCON-8)  1005,1005,1107                                      NTRPD157
 1107 INSC = 1                                                         NTRPD158
      GO TO 246                                                        NTRPD159
 1121 WRITEOUTPUTTAPE6,1122                                            NTRPD160
 1122 FORMAT (48H0 ACCUMULATOR OVERFLOW.  DEN MUST BE TOO SMALL.    )  NTRPD161
      INSC = 1                                                         NTRPD162
      GO TO 246                                                        NTRPD163
      FREQUENCY 1051(1,9),1001(50),1003(50),101(500),1011(50),         NTRPD164
     1  1012(0,0,1),104(50),1043(1,0,1)                                NTRPD165
      END                                                              NTRPD166
```

Table I. (Contd.) UCRL-10925

```
CDGUNC   FINDS G(V) - G(V-X)
      SUBROUTINE DGUNC (XG,DENQ,NGAS,TEMPI)
D     DIMENSION XG(20),DENQ(20)
      DIMENSION UEV(3000),EV(3000),BV(200),BI(3000),TEMP(200),U(200),
     Z          Y(200),Z(200)
      COMMON Y,TEMP,UEV,EV,Q,NST,N,MST,M,XMIN,XMAX,INSC,MBEG,NUST ,BI,
     Z        NI,NS,MAXIT,FACM,ZMU,DE,WE,WEXE,WEYE,WEZE,WETE,BE,ALPHAE,
     Z        GAMMAE,DELTAE,   VNIN,BQ,MQ,SPEP,   U,BV,Z,ICK,H,  K,HDES
     Z        ,EPSLNE
      V = TEMPI
      VA = V*V
      VB = VA*V
      VC = VB*V
  205 DO 210 I = 1,NGAS
D     Y = TEMPI - XG(I)
      X = Y
      XA = X*X
      XB = XA*X
      XC = XB*X
      DENQ(I) = WE*X + (XA-2.*V*X)*WEXE + ((VA*X-V*XA)*3.+XB) * WEYE
     Z          + ((VB*X+V*XB)*4.-6.*VA*XA-XC) * WEZE
     Z          + ((VC*X-V*XC)*5.+(VA*XB-VB*XA)*10.) * WETE
  210 CONTINUE
      RETURN
      END
```

```
CTIME
C     DISCARD THIS SUBROUTINE IF YOUR 709/7090/7094 INSTALLATION HAS
C     AN ON-LINE CLOCK ADDRESSABLE BY CALL TIME(X)
      SUBROUTINE TIME(X)
1     X = 0.0
      RETURN
      END
```

Table II. Sample data deck for RKR program.

```
*      DATA
1
1 RKR PROCEDURE APPLIED TO THE X STATE OF SILICON NITRIDE   TEST PROGRAM
 MOLECULAR CONSTANTS ARE TAKEN FROM JENKINS AND DE LASZLO
   2 9.33526
   1  10    (42H TURNING POINTS ARE GENERATED BY CONSTANTS)
 1151.680  6.560
2
   1  10    (42H TURNING POINTS ARE GENERATED BY CONSTANTS)
 0.7310    0.00567
2
1.5718
0.5        9.5        1.0
```

PROGRAM FOR CALCULATING RELATIVE INTENSITIES

Remarks

The input to this program is extremely flexible. The potential may be generated by subroutine POTGEN or may be read in. The output is Franck-Condon factors, relative intensities (quantum/sec) scaled to ten, relative intensities (energy/sec) scaled to ten, and the off-diagonal matrix elements $\langle v'J' | r | v''J'' \rangle / \langle v'J' | v''J'' \rangle$ and $\langle v'J' | r^2 | v''J'' \rangle / \langle v'J' | v''J'' \rangle$, commonly known as the r-centroid and the square of the r-centroid. The heart of this program is subroutine SCHR which solves the radial Schrödinger equation for its eigenvalues and wavefunctions. This program has been described in detail elsewhere.[3] About 0.9 min is required to calculate all the above-named quantities for ten vibrational levels of the lower state with four vibrational levels of the upper state.[2]

Limitations

Presently the program will calculate at one time the Franck-Condon factors, etc., of only four specified vibrational levels of the upper state with the vibrational levels of the lower state. Also the same (J', J") pair must be used for each transition. This is due to lack of additional space in core storage. The program may be easily modified to allow more flexible usage.

Listing

Table III lists the source decks and Table IV gives a sample data deck for the relative-intensity program.

UCRL-10925

Table III. Source-deck listing for relative-intensity program.

```
CMAIN COMPUTES INTENSITY DISTRIBUTION FOR ELECTRONIC TRANSITIONS.
C      THIS PROGRAM USES D2 NU SCHR AND SIMPSONS RULE TO FIND
C      THE FRANCK CONDON OVERLAP FACTORS AND CORRECTS FOR
C      FREQUENCY DEPENDENCE AND SCALES TO TEN.
C      THE POTENTIAL MAY BE GENERATED INTERNALLY.  OTHERWISE
C       POINTS ON THE POTENTIAL CURVE ARE READ IN.  THEY ARE INTERPOLATED
C       TO ANY DESIRED SPACING (LESS THAN 2000 POINTS).  D2 NU SCHR
C       IS USED TO FIND THE ENERGY LEVELS.  NTRPSR IS USED TO INTERPOLATE
C       THE GIVEN POTENTIAL POINTS.  THE 2 POINTS AT SMALLEST R ARE
C       FITTED EXACTLY TO A FUNCTION OF THE FORM A/X**12+ C.  SIMILARLY
C       THE TWO POINTS AT GREATEST R ARE FITTED EXACTLY TO A FUNCTION OF
C       THE FORM A/X**B.  THESE ARE THEN USED TO EXTRAPOLATE THE
C       POTENTIAL TO THE GIVEN LIMITS.  A SUBROUTINE POTGEN MUST BE
C       INCLUDED.  THIS WILL COMPUTE THE POTENTIAL CURVE OR WILL BE A
C       DUMMY TO SATISFY ENTRY REQUIREMENTS.
C
      DIMENSION XI(200,2),YI(200,2),XO(2000),V(2000,2),S(2000)
     Z          ,SU(2000,4),ETRIAL(200,2)   ,QIRA(2),QIEN(3),QIMS(2)
     Z          ,ZIMS(2),ZIRA(2),ZIEN(3),ECALC(200,2),XPRN(5),VPRN(5)
     Z          ,DTFRMT(10),DUFMT(10),BVF(100,2),RESULT(100,4)
     Z          ,KV(100,2),N(2),NL(2),DE(2),PRFMT(10),PNFT(4)
     Z          ,DIV(4),WE(2),RE(2),RCNTRD(100,4),RRCN(100,4)
     Z          ,DDIV(4)
      COMMON XI,YI,XO,V,XH,NSTA,N,MSTA,M,XMIN,XMAX,INSC,MBEG,NUSED,S,
     Z        NI,NS,MAXIT,FACM,ZMU,DE,WE,WEXE,SU
C
C       THE FOLLOWING COMMENT CARDS DESCRIBE THE PREPARATION OF DATA.
C
C       FIRST CARD IN DATA HAS A ONE IN COLUMN 1 IF A PROBLEM FOLLOWS.
C       VERY LAST CARD IN DATA MUST BE A BLANK CARD.....
C
    1 CALL TIME(BEGIN)
      WRITEOUTPUTTAPE6,160,BEGIN
  160 FORMAT (9H0 TIME =   F10.5)
      READINPUTTAPE5,100,ITEST
  100 FORMAT (I1)
    2 IF (ITEST) 3,400,3
C
C       NEXT  CARD IN DATA HAS NAME OF PROBLEM IN COLUMNS 1-72, WHERE
C       CARRIAGE CONTROL IS IN COLUMN 1.  SECOND CARD HAS IIMS AND
C       MASSES OF THE TWO ATOMS.
C      IF ZMAS2 = 0, ZMAS1 IS TAKEN AS THE REDUCED MASS IN THE IIMS UNITS
C       IIMS = 1, MASS UNITS ARE BASED ON C12 = 12.
C       IIMS = 2, MASS UNITS ARE BASED ON O16 = 16.
C
    3 READINPUTTAPE5,101
  101 FORMAT (72H1 PROBLEM NAME DATE
     Z                                  )
      READINPUTTAPE5,102,IIMS,ZMAS1,ZMAS2
  102 FORMAT (I4,2F10.0)
C
C       NEXT CARD IN DATA HAS IIRA, IIEN, AND THE NUMBER OF POINTS, EACH
C       IN I4 FORMAT, AS WELL AS THE FORMAT STATEMENT WHICH CONTROLS THE
C       READING OF THE POINTS (IN COLUMNS 13-72)--FOR EXAMPLE- (4E16.8).
C       IIEN = 1, ENERGY IS IN ATOMIC UNITS.  (1 A.U. = 27.1961 E.V.)
C       IIEN = 2, ENERGY IS IN 1/CM.
C       IIEN = 3, ENERGY IS IN ELECTRON VOLTS.  ( 1 E.V. = 8065.68 1/CM)
C       IIRA = 1, DISTANCE IS IN ATOMIC UNITS.  ( 1 A.U. = .529166 ANG.)
```

Table III. (Contd.)

```
C        IIRA = 2, DISTANCE IS IN ANGSTROMS.
C        FOLLOWING CARDS CONTAIN THE INPUT POTENTIAL POINTS.
C        IF IT IS DESIRED TO USE A FUNCTION TO GENERATE THE WHOLE
C        POTENTIAL CURVE, THE FIRST 12 COLUMNS OF THE IIRA, ETC. CARD
C        MUST BE BLANK.  A HOLLERITH TEXT MUST BE PUNCHED IN 13-72, AS
C        IT WILL BE PRINTED.  THE NEXT CARD IN SUCH A CASE CONTAINS
C        XMIN,XMAX,ETC.
C       FIRST TIME THROUGH IS THE GROUND STATE
C       THE SECOND TIME THROUGH IS THE UPPER STATE
C       A MAXIMUM OF FOUR LEVELS OF THE UPPER STATE CAN BE USED IN
C       COMPUTING INTENSITIES AT ONE TIME.
C       THE SAME VALUE OF IIEN,IIRA,NDE,XH,XMIN,XMAX,IIRA1,NET
C       ,IIEN1 MUST BE USED FOR BOTH THE GROUND AND UPPER STATE
C
        IKON = 1
      5 READINPUTTAPE5,103,IIRA,IIEN,N(IKON),(DTFRMT(I),I=1,10)
    103 FORMAT (3I4, 10A6)
      6 IF (IIRA) 7,8,7
      7 NIKON = N(IKON)
        READINPUTTAPE5,DTFRMT,(XI(I,IKON),YI(I,IKON),I=1,NIKON)
C
C        NEXT CARD CONTAINS NDE AND THE DISSOCIATION ENERGY WHERE NDE IS
C        ZERO IF ZERO PT OF POTENTIAL CURVE IS AT R=INFINITY, OR ONE IF AT
C        R=REQUILIBRIUM.  DISSOCIATION ENERGY HAS SAME UNITS AS POTENTIAL.
C
        READINPUTTAPE5,105,NDE,DE(IKON)
    105 FORMAT (I4,F10.0)
        GO TO 17
C
C        NEXT DATA CARD CONTAINS XMIN,XMAX,XH,IIRA, WHERE IIRA GIVES THE
C        UNITS FOR THE MIN AND MAX DISTANCES AND THE SPACING XH.
C
      8 READINPUTTAPE5,104,DE(IKON),WE(IKON),RE(IKON)
     17 READINPUTTAPE5,104,XMIN,XMAX,XH,IIRA1
104     FORMAT(3F10.0,I4)
C
C        NEXT CARD HAS NO. AND IIEN OF EXPECTED ENERGY LEVELS, AND NET
C        WHICH HAS THE SAME INTERPRETATION FOR ETRIAL(I) AS NDE DOES FOR
C        THE POTENTIAL CURVE ABOVE.
C       IT ALSO CONTAINS THE VARIABLE FORMAT FOR READING ENERGY LEVELS
C
        READINPUTTAPE5,106,NL(IKON),IIEN1,NET,(DUFMT(I),I=1,10)
    106 FORMAT (3I4, 10A6)
        IF (NL) 15,15,14
     14 NLIKON = NL(IKON)
C
C       READ IN ENERGY LEVELS
C
        READINPUTTAPE5,DUFMT,(KV(I,IKON),ETRIAL(I,IKON),I=1,NLIKON)
C
C       GO BACK TO STATEMENT 5 AND READ IN UPPER STATE
C
     15 GO TO (1501,1502), IKON
   1501 IKON = 2
        GO TO 5
C
C       AFTER BOTH THE LOWER AND UPPER STATES ARE READ IN,
C       D2 NU SCHR MODIFIED FOR THE 709/7090/7094 IS DESCRIBED  IN
```

Table III. (Contd.)

```
C      R. N. ZARE AND J. K. CASHION, UCRL-10881, 1963
C      FOR THIS PROGRAM THE CONSTANTS ARE USED AS FOLLOWS
C      IF NI = 1, PRINTS ITERATIONS, OTHERWISE NOT
C      IF NS = 1, PRINTS WAVEFUNCTION EVERY IPSIQ POINTS, OTHERWISE NOT
C      IF NS = 33, PRINTS EIGENVALUES AND NODE COUNT
C      EPS IS THE CONVERGENCE CRITERION
C      EPS IS IN THE SAME UNITS AS THE POTENTIAL CURVE
C      MAXIT IS THE MAXIMUM NUMBER OF TIMES SCHR WILL TRY TO SATISFY THE
C      CONVERGENCE CRITERION
C
1502   LLIM = 100
       KLIM = 2
       READ INPUT TAPE 5,107,NI,NS,IPSIQ,MAXIT,EPS
107    FORMAT(4I4,E10.0)
C
C      NEXT TWO CARDS ARE THE VALUES OF J FOR THE LOWER AND UPPER STATE
C
       READINPUTTAPE5,144,JROTL,JROTU
144    FORMAT(I3)
C
C      NEXT SIX CARDS ARE THE ROTATIONAL CONSTANTS, BE, ALPHAE, GAMMAE,
C      FOR THE LOWER AND UPPER STATES.
C      THE ROTATIONAL CONSTANTS ARE IN WAVE NUMBERS
C
       READ INPUT TAPE 5,2000,BE1,AE1,GE1,BE2,AE2,GE2
2000   FORMAT(E20.8)
C
C      NEXT DATA CARD CONTAINS TE, OR THE CORRESPONDING QUANTITY IF THE
C      FIRST POTENTIAL IS NOT THE GROUND STATE.  TE IS IN WAVE NUMBERS
C
       READ INPUT TAPE 5,2000,TE
C
C      NEXT CARD CONTAINS NPOT.
C      THE POTENTIAL IS PRINTED AT EVERY NPOT POINT.
C      NPOT = 5 IS SUGGESTED TO THE USER.
C
       READ INPUT TAPE 5,144,NPOT
C
C      THIS TERMINATES COMMENT CARDS ON THE PREPARATION OF DATA.
C      IF NO FURTHER PROBLEMS FOLLOW, REMEMBER TO ADD A BLANK CARD TO THE
C      DATA DECK
C
C
       QIRA(1) = 6HA.U.
       QIRA(2) = 6HANGST.
       QIEN(1) = 6HA.U.
       QIEN(2) = 6H1/CM
       QIEN(3) = 6HE.V.
       QIMS(1) = 6HC12=12
       QIMS(2) = 6HO16=16
       PRFMT(1) = 6H(1H06X
       PRFMT(2) = 6H3HV--4
       PRFMT(3) = 6H(11X5H
       PRFMT(4) = 6HV- = I
       PRFMT(5) = 6H3,11X)
       PRFMT(6) = 3H//)
       PNFT(1)  = 6H3HV--1
       PNFT(2)  = 6H3HV--2
```

Table III. (Contd.)

```
      PNFT(3)   = 6H3HV--3
      PNFT(4)   = 6H3HV--4
C
C     OUTPUT IS IN WAVE NUMBERS AND ANGSTROMS
C      PRINT HEADING
C
      WRITEOUTPUTTAPE6,101
C
C      PRINT THE MASSES AND THEIR UNITS.
C
   10 IF (ZMAS2) 12,12,11
   11 WRITEOUTPUTTAPE6,121,QIMS(IIMS),ZMAS1,ZMAS2
  121 FORMAT (///40H  THE MASSES OF THE TWO ATOMS, BASED ON A6, 6H, ARE
     Z        F10.6, 5H AND  F10.6///)
      GO TO 20
   12 WRITEOUTPUTTAPE6,111,QIMS(IIMS),ZMAS1
  111 FORMAT (///46H  THE REDUCED MASS OF THE TWO ATOMS, BASED ON A6,
     Z         5H, IS  F10.6///)
C
C      PRINT THE INPUT POTENTIAL, THE DISSOCIATION ENERGY, AND UNITS,
C      IF READ IN.
C
      IKON = 1
   20 IF (IIRA) 21,22,21
   21 WRITEOUTPUTTAPE6,122,QIRA(IIRA),QIEN(IIEN)
  122 FORMAT (35H  THE INPUT POTENTIAL POINTS, R IN A6, 15H AND ENERGY I
     ZN  A6, 18H, ARE GIVEN BELOW.  // 1X 5(6X1HR10X1HV4X) //)
      NIKON = N(IKON)
      WRITEOUTPUTTAPE6,114,(XI(I,IKON),YI(I,IKON),I=1,NIKON)
  114 FORMAT (1X F10.6,F12.4,F10.6,F12.4,F10.6,F12.4,F10.6,F12.4,
     Z        F10.6,F12.4)
      WRITEOUTPUTTAPE6,123,DE(IKON)
  123 FORMAT (47H0 DISSOCIATION ENERGY IN SAME UNITS AS ABOVE IS  E20.8)
      GO TO 23
   22 WRITEOUTPUTTAPE6,127
  127 FORMAT (50H  THE POTENTIAL FUNTION IS GENERATED INTERNALLY.   )
      WRITEOUTPUTTAPE6,DTFRMT
C
C      PRINT RMIN, RMAX, THE SPACING, AND THE UNITS.
C
   23 WRITEOUTPUTTAPE6,124,XMIN,XMAX,XH,QIRA(IIRA1)
  124 FORMAT (//// 9H  RMIN = F10.7, 9H, RMAX = F10.7, 12H, SPACING =
     Z         F10.7,  9H, ALL IN  A6)
C
C      PRINT THE TRIAL ENERGY LEVELS AND THEIR UNITS.
C
      IF (NL) 25,25,24
   24 NLIKON = NL(IKON)
      WRITEOUTPUTTAPE6,125,QIEN(IIEN1),(KV(I,IKON),ETRIAL(I,IKON),I=1,NL
     1IKON)
  125 FORMAT (////29H  THE TRIAL ENERGY LEVELS IN A6,16HARE GIVEN BELOW.
     Z        //1X 5(5HLEVEL3X6HENERGY6X)//  (1H  I4,1PE16.7,I4,E16.7,
     Z        I4,E16.7,I4,E16.7,I4,E16.7))
      GO TO 18
25    WRITEOUTPUTTAPE6,161,DE(IKON),WE(IKON),RE(IKON)
  161 FORMAT (7H  DE = F10.2,7H, WE = F10.3,11H, AND RE = F10.6)
C
C      PRINT THE CONVERGENCE CRITERION.
```

Table III. (Contd.)

```
C
   18 GO TO (1801,1802),IKON
 1801 IKON = 2
      GO TO 20
 1802 WRITEOUTPUTTAPE6,126,EPS,QIEN(IIEN)
  126 FORMAT (////43H  CONVERGENCE CRITERION IS ERROR LESS THAN  E9.2,
     Z       2XA6)
C
C       PRINT HEADING
      WRITEOUTPUTTAPE6,101
C
  200 IF (ZMAS2) 201,201,202
  201 ZMU = ZMAS1
      GO TO 204
  202 ZMU = ZMAS1*ZMAS2/(ZMAS1+ZMAS2)
  204 ZIMS(1) = 1.0
      ZIMS(2) = .9996784
      ZIRA(1) = 1.0
      ZIRA(2) = 1.889766
      ZMU = ZMU * ZIMS(IIMS)
      ZIEN(1) = ZMU * 3.643668E3
      ZIEN(2) = ZMU * 1.6610826E-2
      ZIEN(3) = ZMU * 1.339776E2
      FACM = 60.201702/ZMU
      IPOTGN = 0
      N2 = N(2)
      NL2 = NL(2)
  210 IF (IIRA) 214,212,214
C       POTGEN MUST GENERATE THE ENTIRE POTENTIAL CURVE.  IN ADDITION,
C       IT MUST SET THE VALUES OF IIRA,IIEN,M,NDE, AND DE.  NDE WILL BE
C       USED TO SET THE HEIGHT OF THE POTENTIAL CURVE.
  212 CALL POTGEN (IPOTGN,DE,NDE,IIRA,IIEN,RE,ETRIAL,KV,NL,IIEN1,NET,WE,
     1ZMU,XMAX,XMIN,XH,FACM,XO,V,M)
      IF(IPOTGN-10)213,213,1
213   CALL POTGEN(IPOTGN,DE(2),NDE,IIRA,IIEN,RE(2),ETRIAL(1,2),KV(1,2),
     1NL(2),IIEN1,NET,WE(2),ZMU,XMAX,XMIN,XH,FACM,XO,V(1,2),M)
      IF (IPOTGN - 10) 226,226,1
  214 DO 216 I = 1,N
      YI(I) = YI(I)*ZIEN(IIEN)
      XI(I) = XI(I)*ZIRA(IIRA)
  216 CONTINUE
      DE = DE*ZIEN(IIEN)
      DE(2) = DE(2)*ZIEN(IIEN)
  220 DO 222 I = 1,N2
      YI(I,2) = YI(I,2) *ZIEN(IIEN)
      XI(I,2) = XI(I,2)*ZIRA(IIRA)
  222 CONTINUE
  226 XMIN = XMIN*ZIRA(IIRA1)
      XMAX = XMAX*ZIRA(IIRA1)
      XH   = XH  *ZIRA(IIRA1)
      EPS = EPS * ZIEN(IIEN)
      NL2 = NL(2)
      DO 235 I = 1,NL2
      ETRIAL(I,2) = ETRIAL(I,2)*ZIEN(IIEN1)
  235 CONTINUE
  236 DO 238 I = 1,NL
      ETRIAL(I) = ETRIAL(I)*ZIEN(IIEN1)
  238 CONTINUE
```

Table III. (Contd.)

```
C        CHECK FOR RESCALING OF POTENTIAL TO ZERO AT R=INFINITY
  239 IF (NDE) 308,244,240
  240 IF (IPOTGN) 244,241,244
  241 DO 242 I = 1,N
      YI(I) = YI(I) - DE
  242 CONTINUE
      DO 243 I = 1,N2
      YI(I,2) = YI(I,2) - DE(2)
  243 CONTINUE
  244 IF (NET) 300,247,245
  245 DO 246 I = 1,NL
      ETRIAL(I) = ETRIAL(I)-DE+(BE1-AE1*(FLOATF(I-1)+.5)+GE1*(FLOATF(I-1
     1)+.5)**2)*FLOATF(JROTL*(JROTL+1))/FACM
  246 CONTINUE
      DO 2461 I = 1,NL2
      ETRIAL(I,2) = ETRIAL(I,2)-DE(2)+(BE2-AE2*(FLOATF(I-1)+.5)+GE2*(FLO
     1ATF(I-1)+.5)**2)*FLOATF(JROTU*(JROTU+1))/FACM
 2461 CONTINUE
  247 DO 248 I = 1,NL
      ECALC(I) = ETRIAL(I)
  248 CONTINUE
      DO 2481 I = 1,NL2
      ECALC(I,2) = ETRIAL(I,2)
 2481 CONTINUE
      IF(IPOTGN) 250,249,250
  249 NUSED = 8
      CALL TIME(AFTER)
      XTIQ = 60. * (AFTER-BEGIN)
      BEGIN = AFTER
      WRITEOUTPUTTAPE6,131,XTIQ
  131 FORMAT (23H0 TIME BEFORE POTFIT =   F10.5)
      IKON = 1
 2490 CALL POTFIT(XI(1,IKON),YI(1,IKON),N(IKON),XO,V(1,IKON),M,XH,
     Z             XMIN,XMAX,INSC,NUSED,FACM)
      IF (INSC) 1,2491,1
 2491 CALL TIME(AFTER)
      XTIQ = 60. * (AFTER-BEGIN)
      BEGIN = AFTER
      WRITEOUTPUTTAPE6,132,XTIQ
  132 FORMAT (20H0 TIME FOR POTFIT =  F10.5)
C
C        PRINT THE POTENTIAL CURVE GENERATED (ANGSTROMS AND 1/CM)
  250 WRITEOUTPUTTAPE6,108
  108 FORMAT (37H0 THE POTENTIAL FUNCTION GENERATED IS ///
     Z          1X 5(3X 4HR(A) 6X 7HV(1/CM) 2X))
  252 NPOT4 = NPOT*4
      NPOT5 = NPOT*5
  254 DO 270 I = 1,M,NPOT5
  256 IF (M-I-NPOT4) 258,262,262
  258 JFIN = (M-I)/NPOT
  260 IF (JFIN) 272,272,264
  262 JFIN = 5
  264 DO 266 J = 1,JFIN
      IPRN = I + NPOT*(J-1)
      XPRN(J) = XO(IPRN)*.529166
      VPRN(J) = (V(IPRN,IKON)+DE(IKON))*FACM
  266 CONTINUE
      IF (VPRN(1) - 1.E6) 268,269,269
```

Table III. (Contd.)

```
  269 WRITEOUTPUTTAPE6,141,(XPRN(J),VPRN(J),J=1,JFIN),IPRN
  141 FORMAT (1X0PF10.6,1PE12.5,4(0PF10.6,1PE12.5),4XI5)
      GO TO 270
  268 WRITEOUTPUTTAPE6,109,(XPRN(J),VPRN(J),J=1,JFIN),IPRN
  109 FORMAT (1X F10.6,F12.4,F10.6,F12.4,F10.6,F12.4,F10.6,F12.4,
     Z          F10.6,F12.4,4XI5)
  270 CONTINUE
  272 CALL TIME(AFTER)
      XTIQ = 60. * (AFTER-BEGIN)
      BEGIN = AFTER
      WRITEOUTPUTTAPE6,135,XTIQ
  135 FORMAT (32H0 TIME FOR PRINT OF POTENTIAL = F9.4,9H SECONDS.)
      GO TO (2721,2729), IKON
 2721 IKON = 2
      WRITEOUTPUTTAPE6,101
      GO TO 2490
 2729 DO 2728 J = 1,M
      V(J,1) = FLOATF(JROTL*(JROTL+1))/XO(J)**2+V(J,1)
      IF ACCUMULATOR OVERFLOW 2724,2725
 2724 V(J,1) = 1.0E+30
 2725 V(J,2) = FLOATF(JROTU*(JROTU+1))/XO(J)**2+V(J,2)
      IF ACCUMULATOR OVERFLOW 2727,2728
 2727 V(J,2) = 1.0E+30
 2728 CONTINUE
 2722 MTEMQ = M
      LLK = 0
      KLK = 0
C       FIND THE ENERGY LEVELS THROUGH USE OF SCHR.
  274 NLIKON = NL(IKON)
      DO 285 I = 1,NLIKON
  276 IF (SCHR(NI,NS,MAXIT,EPS,IPSIQ,V(1,IKON),XO,S ,M       ,XMIN,
     Z           XMAX,KV(I,IKON),ECALC(I,IKON),FACM)-1.) 284,278,300
  278 LLK = LLK + 1
  280 IF (LLK-LLIM) 284,284,304
  284 M = MTEMQ
      DO 281 J = 1,M
      XO(J) = FLOATF(J-1)*XH + XMIN
  281 CONTINUE
      BVSUM = S(1)**2/XO(1)**2 + 4.*S(2)**2/XO(2)**2 + S(M)**2/XO(M)**2
      KSIMP = M - 1
      DO 287 J = 3,KSIMP,2
      BVSUM = 2.*S(J)**2/XO(J)**2 + 4.*S(J+1)**2/XO(J+1)**2 + BVSUM
  287 CONTINUE
      GO TO (2875,2871), IKON
 2871 DO 2872 J = 1,M
      SU(J,I) = S(J)
 2872 CONTINUE
      GO TO 2878
 2875 DO 2877 IK = 1,NL2
      DO 2876 J = 1,M
      XO(J) = (FLOATF(J-1)*XH+XMIN)*SU(J,IK)
 2876 CONTINUE
 2879 CONTINUE
      CALL SIMP(S,SU(1,IK),M,XH,RESULT(I,IK))
      CALL SIMP(S,XO,M,XH,RCNTRD(I,IK))
 2877 CONTINUE
      DO 2882 IK = 1,NL2
      DO 2881 J = 1,M
```

Table III. (Contd.)

```
      XO(J) = (FLOATF(J-1)*XH+XMIN)**2*SU(J,IK)
2881  CONTINUE
      CALL SIMP(S,XO,M,XH,RRCN(I,IK))
2882  CONTINUE
 2878 BVF(I,IKON) = FACM * BVSUM * XH / 3.
      ECALC(I,IKON) = DE(IKON) * FACM + ECALC(I,IKON)
      CALL TIME(AFTER)
      XTIQ = 60. * (AFTER-BEGIN)
      BEGIN = AFTER
      WRITEOUTPUTTAPE6,162,ECALC(I,IKON),BVF(I,IKON),XTIQ
  162 FORMAT (30H0 SCHR FINDS ENERGY LEVEL G = F11.5,15H 1/CM AND BV =
     Z        F11.7,9H 1/CM IN F7.4,9H SECONDS. )
  285 CONTINUE
      GO TO (2852,2851),IKON
 2851 IKON = 1
      GO TO 2722
 2852 WRITEOUTPUTTAPE6,101
      WRITEOUTPUTTAPE6,110,LLK
  110 FORMAT (38H0 PROGRAM SUCCESSFUL. (MAXIT REACHED  I2, 7H TIMES)  )
      WRITEOUTPUTTAPE6,128
  128 FORMAT (35H0 THE BELOW IS FOR THE LOWER STATE. )
      WRITEOUTPUTTAPE6,133
  133 FORMAT (54H0VIB. NO.   GIVEN ENERGY  CALC. ENERGY      DIFFERENCE
     Z         13X43HGIVEN DELTA G  CALC. DELTA G     DIFFERENCE /44X
     Z         26HDIFFERENCE = CALC. - GIVEN //)
  286 DO 288 I = 1,NL
      ETRIAL(I) = (ETRIAL(I) + DE) * FACM
      DIFF = ECALC(I) - ETRIAL(I)
      IF (I-1) 290,290,292
  292 DGT = ETRIAL(I) - ETRIAL(I-1)
      DGC = ECALC(I) - ECALC(I-1)
      DIFDE = DGC - DGT
      WRITEOUTPUTTAPE6,136,DGT,DGC,DIFDE
  136 FORMAT (    64X3F15.5)
  290 WRITEOUTPUTTAPE6,134,KV(I),ETRIAL(I),ECALC(I),DIFF
  134 FORMAT (I8, 3F15.5)
  288 CONTINUE
      WRITEOUTPUTTAPE6,130
  130 FORMAT (1H128X8HVIB. NO.3X9HCALC.  BV //)
      DO 294 I = 1,NL
      WRITEOUTPUTTAPE6,129,KV(I),BVF(I)
  129 FORMAT (28XI7,3F15.8)
  294 CONTINUE
      WRITEOUTPUTTAPE6,101
      WRITEOUTPUTTAPE6,137
  137 FORMAT (35H0 THE BELOW IS FOR THE UPPER STATE. )
      WRITEOUTPUTTAPE6,138
  138 FORMAT (54H0VIB. NO.   GIVEN ENERGY  CALC. ENERGY      DIFFERENCE
     Z         /44X26HDIFFERENCE = CALC. - GIVEN //)
      DO 388 I = 1,NL2
      ETRIAL(I,2) = (ETRIAL(I,2) + DE(2)) * FACM
      DIFF = ECALC(I,2)-ETRIAL(I,2)
      WRITEOUTPUTTAPE6,134,KV(I,2),ETRIAL(I,2),ECALC(I,2),DIFF
  388 CONTINUE
      WRITEOUTPUTTAPE6,130
      DO 394 I = 1,NL2
      WRITEOUTPUTTAPE6,129,KV(I,2),BVF(I,2)
  394 CONTINUE
```

Table III. (Contd.)

```
      DO 510 J = 1,NL
      DO 510 IK = 1,NL2
      RCNTRD(J,IK) = RCNTRD(J,IK)*0.529166/RESULT(J,IK)
      RRCN(J,IK) = RRCN(J,IK)*0.529166**2/RESULT(J,IK)
      RESULT(J,IK) = RESULT(J,IK)**2
510   CONTINUE
      WRITE OUTPUT TAPE 6,500
500   FORMAT(24H1 FRANCK-CONDON FACTORS       )
      PRFMT(2) = PNFT(NL2)
      WRITE OUTPUT TAPE 6,PRFMT,(KV(J,2),J = 1,NL2)
      DO 520 J = 1,NL
      WRITE OUTPUT TAPE 6,508,KV(J),(RESULT(J,ILK),ILK = 1,NL2)
508   FORMAT(6X,I4,4(10X,E10.4,10X))
520   CONTINUE
      WRITE OUTPUT TAPE 6,514
514   FORMAT(32H1 R-CENTROID FACTORS (ANGSTROMS)  )
      WRITE OUTPUT TAPE 6,PRFMT,(KV(J,2),J = 1,NL2)
      DO 516 J = 1,NL
      WRITE OUTPUT TAPE 6,508,KV(J),(RCNTRD(J,ILK),ILK = 1,NL2)
516   CONTINUE
      WRITE OUTPUT TAPE 6,517
517   FORMAT(17H1 R**2-CENTROIDS   )
      WRITE OUTPUT TAPE 6,PRFMT,(KV(J,2),J = 1,NL2)
      DO 518 J = 1,NL
      WRITE OUTPUT TAPE 6,508,KV(J),(RRCN(J,ILK),ILK = 1,NL2)
518   CONTINUE
C
C     CORRECT FOR FREQUENCY DEPENDENCE
C     AND SCALE TO TEN
C
      DO 5121 IK = 1,NL2
      DIV(IK) = 0.0
      DDIV(IK) = 0.0
      DO 5121 J = 1,NL
      RESULT(J,IK) = RESULT(J,IK)   *(TE+ECALC(IK,2)-ECALC(J,1))**3
      RCNTRD(J,IK) = RESULT(J,IK)*(TE+ECALC(IK,2)-ECALC(J,1))
5121  CONTINUE
      DO 5022 IK = 1,NL2
      DO 5022 J = 1,NL
      DIV(IK) = MAX1F(DIV(IK),RESULT(J,IK))
      DDIV(IK) = MAX1F(DDIV(IK),RCNTRD(J,IK))
5022  CONTINUE
      DO 5023 IK = 1,NL2
      DO 5023 J = 1,NL
      RESULT(J,IK) = RESULT(J,IK)/DIV(IK)*10.0
      RCNTRD(J,IK) = RCNTRD(J,IK)/DDIV(IK)*10.0
5023  CONTINUE
      WRITE OUTPUT TAPE 6,5024
5024  FORMAT(48H1 RELATIVE INTENSITY(QUANTUM/SEC) SCALED TO TEN  )
      WRITE OUTPUT TAPE 6,PRFMT,(KV(J,2),J = 1,NL2)
      DO 5026 J = 1,NL
      WRITE OUTPUT TAPE 6,509,KV(J),(RESULT(J,ILK),ILK = 1,NL2)
509   FORMAT(6X,I4,4(12X,F6.3,12X))
5026  CONTINUE
      WRITE OUTPUT TAPE 6,5030
5030  FORMAT(47H1 RELATIVE INTENSITY(ENERGY/SEC) SCALED TO TEN  )
      WRITE OUTPUT TAPE 6,PRFMT,(KV(J,2),J = 1,NL2)
      DO 5027 J = 1,NL
```

Table III. (Contd.)

```
      WRITE OUTPUT TAPE 6,509,KV(J),(RCNTRD(J,ILK),ILK = 1,NL2)           MAIN 522
 5027 CONTINUE                                                            MAIN 523
      WRITE OUTPUT TAPE 6,5031                                            MAIN 524
 5031 FORMAT(12H1 CONSTANTS )                                             MAIN 525
      WRITE OUTPUT TAPE 6,144,JROTL,JROTU                                 MAIN 526
      WRITE OUTPUT TAPE 6,2000,TE,BE1,BE2,AE1,AE2,GE1,GE2                 MAIN 527
      GO TO 1                                                             MAIN 528
  300 KLK = KLK + 1                                                       MAIN 529
  301 IF (KLK-KLIM) 284,302,302                                           MAIN 530
  302 WRITEOUTPUTTAPE6,112,KLIM                                           MAIN 531
  112 FORMAT (26H0 SCHR NOT SUCCESSFUL FOR I2, 28HTH TIME, GO TO NEXT PRMAIN 532
     ZOBLEM.   )                                                          MAIN 533
      GO TO 1                                                             MAIN 534
  304 WRITEOUTPUTTAPE6,113,LLIM,I                                         MAIN 535
  113 FORMAT (28H0 SCHR DID NOT CONVERGE FOR I2,17HTH TIME WHEN I = I3)   MAIN 536
  306 GO TO 1                                                             MAIN 537
  308 WRITEOUTPUTTAPE6,120,NDE                                            MAIN 538
  120 FORMAT (25H0 ERROR IN INPUT.  NDE =     I10)                        MAIN 539
      GO TO 1                                                             MAIN 540
  400 CALL EXIT                                                           MAIN 541
      END                                                                 MAIN 542
```

```
CPOTFIT  USING NTRPSR,MINFIT,MAXFIT                                       POTFT000
      SUBROUTINE POTFIT (XI,YI,N,XO,V,M,XH,XMIN,XMAX,INSC,NUSED,FACM)     POTFT001
      DIMENSION XI(400),YI(400),XO(2000),V(2000)                          POTFT002
  248 MBEG = 1                                                            POTFT003
      XMAXT = XMAX                                                        POTFT004
      XMINT = XMIN                                                        POTFT005
C       CHECK FOR EXTRAPOLATION AT SMALL R.                               POTFT006
  250 IF (XMIN - XI(1)) 252,254,254                                       POTFT007
  252 XMAX  = XI(1)                                                       POTFT008
      CALL MINFIT (XI,YI,N,XO,V,M,XH,XMIN,XMAX,INSC,FACM)                 POTFT009
      IF (INSC) 712,253,712                                               POTFT010
  253 MT = M                                                              POTFT011
      XMIN = XO(MT) + XH                                                  POTFT012
      MBEG = M + 1                                                        POTFT013
C       PREPARE TO INTERPOLATE.                                           POTFT014
  254 M = 0                                                               POTFT015
      XMAX = XMAXT                                                        POTFT016
      NL = N-1                                                            POTFT017
  256 IF ( XMAX-XI(NL))260,260,258                                        POTFT018
  258 XMAX = XI(NL)                                                       POTFT019
  260 CALL NTRPSR(XI,YI,XO,V,XH,N,M,XMIN,XMAX,INSC,MBEG,NUSED)            POTFT020
C       CHECK FOR EXTRAPOLATION AT LARGE R.                               POTFT021
      IF (INSC) 712,262,712                                               POTFT022
  262 IF (XMAXT-XMAX) 267,267,264                                         POTFT023
  264 MBEG = M + MBEG                                                     POTFT024
      XMIN = XO(MBEG-1) + XH                                              POTFT025
      XMAX = XMAXT                                                        POTFT026
  266 CALL MAXFIT (XI,YI,N,XO,V,M,XH,XMIN,XMAX,INSC,FACM,MBEG)            POTFT027
  267 XMIN = XMINT                                                        POTFT028
      M = M + MBEG - 1                                                    POTFT029
  712 RETURN                                                              POTFT030
      END                                                                 POTFT031
```

Table III. (Contd.)

```
CMINFIT         Y = A/X**12+ C                                                  MINFT000
      SUBROUTINE MINFIT (X,Y,N,XO,V,M,XH,XMIN,XMAX,INSC,FACM)                   MINFT001
      DIMENSION X (400),Y (400),XO(2000),V(2000)                                MINFT002
      R12FUF(X) = A/X**12 + C                                                   MINFT003
      M = XFIXF((XMAX-XMIN)/XH) + 1                                             MINFT004
      A = (Y(1)-Y(2))/(1./X(1)**12 - 1./X(2)**12)                               MINFT005
      C = Y(1) - A/X(1)**12                                                     MINFT006
  212 DO 214 I = 1,M                                                            MINFT007
      XO(I) = FLOATF(I-1)*XH + XMIN                                             MINFT008
      V (I) = R12FUF(XO(I))                                                     MINFT009
  214 CONTINUE                                                                  MINFT010
      A = A*FACM*.529166**12                                                    MINFT011
      C = C*FACM                                                                MINFT012
      WRITEOUTPUTTAPE6,101,A,C                                                  MINFT013
  101 FORMAT (70H0 LEFT END OF POTENTIAL FUNCTION IS FOUND FROM Y=A/X**1MINFT014
     22+C, WHERE A =  1PE14.7, 9H AND C = E14.7  )                              MINFT015
      RETURN                                                                    MINFT016
      END                                                                       MINFT017
```

```
CMAXFIT         Y = A/X**B                                                      MAXFT000
      SUBROUTINE MAXFIT (X,Y,N,XO,V,M,XH,XMIN,XMAX,INSC,FACM,MBEG)              MAXFT001
      DIMENSION X (400),Y (400),XO(2000),V(2000)                                MAXFT002
      R6FUNF(X) = A/X**B                                                        MAXFT003
      L = N - 1                                                                 MAXFT004
      B = LOGF(Y(L)/Y(N))/LOGF(X(N)/X(L))                                       MAXFT005
      A = Y(N) * X(N)**B                                                        MAXFT006
      M = XFIXF((XMAX-XMIN)/XH) + 1                                             MAXFT007
      MFIN = MBEG + M - 1                                                       MAXFT008
  202 DO 204 I = MBEG,MFIN                                                      MAXFT009
      XO(I) = FLOATF(I-MBEG)*XH + XMIN                                          MAXFT010
      V(I) = R6FUNF(XO(I))                                                      MAXFT011
  204 CONTINUE                                                                  MAXFT012
      A = A*FACM*.529166**B                                                     MAXFT013
      WRITEOUTPUTTAPE6,206,A,B                                                  MAXFT014
  206 FORMAT (68H0 RIGHT END OF POTENTIAL FUNCTION IS FOUND FROM Y=A/X**MAXFT015
     ZB, WHERE A = E14.7,  9H AND B =  E14.7)                                   MAXFT016
      RETURN                                                                    MAXFT017
      END                                                                       MAXFT018
```

Table III. (Contd.)

```
CNTRPSR  INTERPOLATION PROGRAM (BY SUCCESSIVE RANGES)  SINGLE PREC.
C
C       THE METHOD OF LAGRANGE IS USED.  THE INPUT POINTS NEED NOT BE
C       EQUALLY SPACED.  THERE ARE TWO MODES OF INPUT AVAILABLE.  THE
C       FIRST OCCURS WHEN M = 0.  THE ABSCISSAE ARE THEN GENERATED FROM
C       XMIN,XMAX,AND XH.  AT EXIT M = NO. OF POINTS FOUND, AND XO
C       CONTAINS THE ABSCISSAE.  M WILL BE CHECKED TO INSURE THAT THE
C       DIMENSION IS NOT EXCEEDED.  MDIMM = THE DIMENSION OF THE XO, YO
C       ARRAYS.  THE SECOND MODE OCCURS WHEN M IS POSITIVE.  THE M
C       ABSCISSAE ARE THEN ASSUMED TO HAVE BEEN GENERATED PRIOR TO
C       ENTRY.  THE STARTING INDEX FOR THE OUTPUT ARRAY MUST BE
C       SPECIFIED.  THE FIRST POINT FOUND WILL BE AT XO(MBEG).  XH MUST
C       BE GIVEN SINCE THE ORDINATE FOR ANY POINT CLOSER THAN .01*XH TO
C       AN INPUT POINT IS TAKEN AS THAT FOR THE INPUT POINT.  -NUSED- IS
C       THE NUMBER OF POINTS USED FOR EACH INTERPOLATED POINT.  *NUSED*
C       MUST BE EVEN AND LESS THAN OR EQUAL TO -N-.  NUSED = 8 IS
C       SUGGESTED.  ANY POINT FARTHER THAN NUSED/2 POINTS FROM EITHER END
C       IS FOUND FROM THE NUSED/2 ON EACH SIDE.  NTRPSR WILL SCALE AND
C       RESCALE IN ORDER TO AVOID OVERFLOW.  IF THE FIRST SCALING DOES
C       NOT SUCCEED, NTRPSR WILL TRY UP TO 7 TIMES MORE BEFORE RETURNING
C       IN THE ERROR MODE. (INSC = 1)
C       INPUT IS  XI,YI,(XO),XH,N,M,(XMIN),(XMAX),MBEG,NUSED.
C       OUTPUT IS  (XO),YO,INSC.
C       INSC = 0 IF PROGRAM WAS SUCCESSFUL.  IF NOT, INSC = 1.
C
      SUBROUTINE NTRPSR(XJ,YJ,XO,YO,XN,N,K,XNIN,XNAX,INSC,MBEG,NUSED)
      DIMENSION XI(400),YI(400),XO(2000),YO(2000),XJ(400),YJ(400),NUMB(4
     100)
      MDIMM = 2000
      XMAX = XNAX
      XMIN = XNIN
      XH = ABSF(XN)
      M = K
      IREV = 0
      IREX = 0
C     M IS ZERO, IF XH, XMIN, XMAX ARE TO BE USED.  IF M IS NOT = TO
C     ZERO, THEN XO(I), I = 1,M WILL BE USED AS ABSCISSA.
  200 IF (M) 270,201,206
  201 M = XINTF(ABSF((XMAX-XMIN)/XH)) + 1
C     IF M IS MORE THAN DIMENSION OF XO, RETURN IN ERROR MODE.
      IF (M+MBEG-MDIMM-2) 202,272,272
  202 MF = MBEG + M - 1
      IF (XMAX - XMIN) 203,204,204
  203 XMIN = XNAX
      XMAX = XNIN
      IREV = 1
  204 DO 205 I = MBEG,MF
      XO(I) = FLOATF(I-MBEG) * XH + XMIN
  205 CONTINUE
  206 DO 207 I = 1,N
      XI(I) = XJ(I)
  207 CONTINUE
      MF = MBEG + M - 1
      MSTA = MBEG
      NUST = NUSED/2
      NS = NUST + 1
      NF = N - NS + 1
      NFP = NF + 1
```

Table III. (Contd.)

```
      DO 208 I = NS,NFP                                                 NTRPS058
      NUMB(I) = 0                                                       NTRPS059
  208 CONTINUE                                                          NTRPS060
      IF (XO(MF) - XO(MBEG)) 209,211,211                                NTRPS061
  209 M2 = M/2                                                          NTRPS062
      M2F = MBEG + M2 - 1                                               NTRPS063
      DO 210 I = MBEG,M2F                                               NTRPS064
      K = MF + MBEG - I                                                 NTRPS065
      TEMP = XO(I)                                                      NTRPS066
      XO(I) = XO(K)                                                     NTRPS067
      XO(K) = TEMP                                                      NTRPS068
  210 CONTINUE                                                          NTRPS069
      IREV = 1                                                          NTRPS070
  211 IF (XI(N)-XI(1)) 212,216,216                                      NTRPS071
  212 N2 = N/2                                                          NTRPS072
      DO 214 I = 1,N2                                                   NTRPS073
      K = N + 1 - I                                                     NTRPS074
      TEMP = XJ(I)                                                      NTRPS075
      TEMS = YJ(I)                                                      NTRPS076
      XJ(I) = XJ(K)                                                     NTRPS077
      YJ(I) = YJ(K)                                                     NTRPS078
      XJ(K) = TEMP                                                      NTRPS079
      YJ(K) = TEMS                                                      NTRPS080
  214 CONTINUE                                                          NTRPS081
      IREX = 1                                                          NTRPS082
  216 IF (NF-NS) 236,218,218                                            NTRPS083
  218 DO 226 J = MBEG,MF                                                NTRPS084
      DO 224 I = NS,NF                                                  NTRPS085
  220 IF(XO(J)-XJ(I))222,222,224                                        NTRPS086
  222 NUMB(I) = NUMB(I) + 1                                             NTRPS087
      GO TO 226                                                         NTRPS088
  224 CONTINUE                                                          NTRPS089
      NUMB(NFP) = NUMB(NFP) + 1                                         NTRPS090
  226 CONTINUE                                                          NTRPS091
      GO TO 238                                                         NTRPS092
  236 NUMB(NFP) = M                                                     NTRPS093
  238 M = 0                                                             NTRPS094
  239 DO 250 L = NS,NFP                                                 NTRPS095
      IF (NUMB(L)) 250,250,242                                          NTRPS096
  242 M = NUMB(L)                                                       NTRPS097
      NSTA = L - NUST                                                   NTRPS098
      GO TO 100                                                         NTRPS099
  246 IF (INSC) 274,248,274                                             NTRPS100
  248 MSTA = MSTA + M                                                   NTRPS101
  250 CONTINUE                                                          NTRPS102
  240 K = MSTA - MBEG                                                   NTRPS103
      IF (IREV) 256,256,252                                             NTRPS104
  252 M2F = K/2 + MBEG - 1                                              NTRPS105
      DO 254 I = MBEG,M2F                                               NTRPS106
      J = MF + MBEG - I                                                 NTRPS107
      TEMP = XO(I)                                                      NTRPS108
      TEMS = YO(I)                                                      NTRPS109
      XO(I) = XO(J)                                                     NTRPS110
      YO(I) = YO(J)                                                     NTRPS111
      XO(J) = TEMP                                                      NTRPS112
      YO(J) = TEMS                                                      NTRPS113
  254 CONTINUE                                                          NTRPS114
  256 IF (IREX) 262,262,258                                             NTRPS115
```

Table III. (Contd.)

```
  258 DO 260 I = 1,N2                                                   NTRPS116
      J = N + 1 - I                                                     NTRPS117
      TEMP = XJ(I)                                                      NTRPS118
      TEMS = YJ(I)                                                      NTRPS119
      XJ(I) = XJ(J)                                                     NTRPS120
      YJ(I) = YJ(J)                                                     NTRPS121
      XJ(J) = TEMP                                                      NTRPS122
      YJ(J) = TEMS                                                      NTRPS123
  260 CONTINUE                                                          NTRPS124
  262 RETURN                                                            NTRPS125
  270 WRITEOUTPUTTAPE6,2101                                             NTRPS126
 2101 FORMAT (44H0 ERROR IN INPUT TO NTRPSR.  M IS NEGATIVE.    )       NTRPS127
      INSC = 1                                                          NTRPS128
      GO TO 240                                                         NTRPS129
  272 H = (XMAX-XMIN)/FLOATF(MDIMM-MBEG)                                NTRPS130
      WRITEOUTPUTTAPE6,2102,H                                           NTRPS131
 2102 FORMAT (58H0 ERROR IN INPUT TO NTRPSR.  MINIMUM ALLOWABLE SPACING NTRPS132
     8IS     1PE12.3)                                                   NTRPS133
      INSC = 1                                                          NTRPS134
      GO TO 240                                                         NTRPS135
  274 WRITEOUTPUTTAPE6,2103,L                                           NTRPS136
 2103 FORMAT (43H0 INTR1 WAS UNABLE TO INTERPOLATE IN RANGE    I3)      NTRPS137
      GO TO 240                                                         NTRPS138
  100 NCON = 1                                                          NTRPS139
      REFA = 1.414214                                                   NTRPS140
      NFIN = NSTA + NUSED - 1                                           NTRPS141
      DO 98 I = NSTA,NFIN                                               NTRPS142
      XI(I) = XJ(I)                                                     NTRPS143
      YI(I) = YJ(I)                                                     NTRPS144
   98 CONTINUE                                                          NTRPS145
      NSTA1 = NSTA + 1                                                  NTRPS146
      XSCALE = (XI(NFIN) - XI(NSTA))/10.                                NTRPS147
      IF (XSCALE) 995,991,995                                           NTRPS148
  991 XSCALE = 1.                                                       NTRPS149
  995 YMAX = YI(NSTA)                                                   NTRPS150
      YMIN = YI(NSTA)                                                   NTRPS151
 1001 DO 1002 I = NSTA1,NFIN                                            NTRPS152
      YMAX = MAX1F(YMAX,YI(I))                                          NTRPS153
      YMIN = MIN1F(YMIN,YI(I))                                          NTRPS154
 1002 CONTINUE                                                          NTRPS155
   91 YSCALE = YMAX - YMIN                                              NTRPS156
      IF (YSCALE) 915,915,1003                                          NTRPS157
  915 YSCALE = 1.                                                       NTRPS158
 1003 DO 1004 I = NSTA,NFIN                                             NTRPS159
      XI(I) = XI(I)/XSCALE                                              NTRPS160
      YI(I) = (YI(I)-YMIN)/YSCALE + .5                                  NTRPS161
 1004 CONTINUE                                                          NTRPS162
      XH = ABSF(XN)/XSCALE                                              NTRPS163
      MFIN = MSTA + M - 1                                               NTRPS164
      MTA = MSTA                                                        NTRPS165
 1005 EPSIL = .01*XH                                                    NTRPS166
  101 DO 110 II=  MTA,MFIN                                              NTRPS167
      XO(II) = XO(II)/XSCALE                                            NTRPS168
      YO(II) = 0.0                                                      NTRPS169
      PNUM = 1.0                                                        NTRPS170
 1011 DO 107 I = NSTA,NFIN                                              NTRPS171
C     FIND XO(II)-XI(I) FOR NUMERATOR AND CHECK FOR NEARNESS.           NTRPS172
      XNUM     = XO(II) - XI(I)                                         NTRPS173
```

Table III. (Contd.)

```
 1012 IF (ABSF(XNUM    )-EPSIL) 102,102,103                              NTRPS174
  102 YO(II) = YI(I)                                                     NTRPS175
      GO TO 109                                                          NTRPS176
C     PNUM = PRODUCT OF ALL XNUM                                         NTRPS177
  103 PNUM = PNUM*XNUM                                                   NTRPS178
C     CONSTRUCT DENOMINATOR AND SUM                                      NTRPS179
      PDEN = 1.0                                                         NTRPS180
  104 DO 106 J = NSTA,NFIN                                               NTRPS181
 1043 IF (I-J) 105,106,105                                               NTRPS182
  105 PDEN =        (XI(I) - XI(J))*PDEN                                 NTRPS183
 1051 IF QUOTIENT OVERFLOW 1103,106                                      NTRPS184
  106 CONTINUE                                                           NTRPS185
      DEN = PDEN*XNUM                                                    NTRPS186
      YO(II) = YI(I)/DEN + YO(II)                                        NTRPS187
      IF ACCUMULATOR OVERFLOW  1121, 107                                 NTRPS188
  107 CONTINUE                                                           NTRPS189
      YO(II) = YO(II)*PNUM                                               NTRPS190
  109 YO(II) = (YO(II)-.5)*YSCALE + YMIN                                 NTRPS191
      XO(II) = XO(II) * XSCALE                                           NTRPS192
  110 CONTINUE                                                           NTRPS193
      INSC = 0                                                           NTRPS194
      GO TO 246                                                          NTRPS195
 1103 WRITEOUTPUTTAPE6,1104,NCON,XSCALE                                  NTRPS196
      WRITEOUTPUTTAPE6,1108,II,I,J                                       NTRPS197
 1104 FORMAT (8H  NCON = I3, 11H, XSCALE =   F10.7)                      NTRPS198
 1108 FORMAT (26H  OVERFLOW OCCURRED AT II= I4,4H  I= I3,4H  J= I3)      NTRPS199
      NCON = NCON + 1                                                    NTRPS200
 1105 DO 1106 I = NSTA,NFIN                                              NTRPS201
      XI(I) = XI(I)/REFA                                                 NTRPS202
 1106 CONTINUE                                                           NTRPS203
      XO(II) = XO(II) * XSCALE                                           NTRPS204
      MTA = II                                                           NTRPS205
      XH   = XH  /REFA                                                   NTRPS206
      XSCALE = XSCALE*REFA                                               NTRPS207
      IF (NCON-8)  1005,1005,1107                                        NTRPS208
 1107 INSC = 1                                                           NTRPS209
      GO TO 246                                                          NTRPS210
 1121 WRITEOUTPUTTAPE6,1122                                              NTRPS211
 1122 FORMAT (48H0 ACCUMULATOR OVERFLOW.  DEN MUST BE TOO SMALL.    )    NTRPS212
      INSC = 1                                                           NTRPS213
      GO TO 246                                                          NTRPS214
      FREQUENCY 1051(1,9),1001(50),1003(50),101(500),1011(50),           NTRPS215
     1  1012(0,0,1),104(50),1043(1,0,1)                                  NTRPS216
      END                                                                NTRPS217
```

Table III. (Contd.)

```
CSIMP                                                                   SIMPS000
C     INTEGRATION OF A PRODUCT S*SS BY SIMPSONS RULE.                   SIMPS001
      SUBROUTINE SIMP(S,SS,N,H,RESULT)                                  SIMPS002
      DIMENSION S(2000),SS(2000)                                        SIMPS003
      SUM = 0.0                                                         SIMPS004
      DO 1 J = 2,N,2                                                    SIMPS005
1     SUM = SUM + 2.0*S(J)*SS(J) + 4.0*S(J-1)*SS(J-1)                   SIMPS006
      RESULT = SUM*H/3.0                                                SIMPS007
      RETURN                                                            SIMPS008
      END                                                               SIMPS009
```

```
CTIME                                                                   TIME 000
C     DISCARD THIS SUBROUTINE IF YOUR 709/7090/7094 INSTALLATION HAS    TIME 001
C     AN ON-LINE CLOCK ADDRESSABLE BY CALL TIME(X)                      TIME 002
      SUBROUTINE TIME(X)                                                TIME 003
1     X = 0.0                                                           TIME 004
      RETURN                                                            TIME 005
      END                                                               TIME 006
```

```
CPOTGEN     THIS IS A DUMMY SUBROUTINE                                  POTGN000
C     POTGEN GENERATES THE POTENTIAL.                                   POTGN001
      SUBROUTINE POTGEN(IPOTGN,DE,NDE,IIRA,IIEN,RE,ETRIAL,KV,NL,IIEN1,  POTGN002
     Z                  NET,WE,ZMU,XMAX,XMIN,XH,FACM,XO,V,M)            POTGN003
1     IPOTGN = 10                                                       POTGN004
      RETURN                                                            POTGN005
      END                                                               POTGN006
```

Table III. (Contd.)

```
CSCHRV   PRINTS EVERY -IPSIQ-TH POINT OF THE WAVE FUNCTIONS.
C      RADIAL SOLUTION TO SCHRODINGER EQUATION SUBROUTINE
       FUNCTION SCHR (NI,NS,MAXIT,EPS,IPSIQ,V,P,S,N,RMIN,RMAX,KV,E0,FACM)
       DIMENSION V(2000,2),S(2000),P(2000),Y(3)
C       USE UNITS SUCH THAT SCHR EQN IS-PSI2 + (E-V)PSI = 0
C      NI=1, PRINT ITERATIONS
C      NI=OTHERWISE, DONT PRINT
C      NS=1, PRINT SOLUTIONS WITH EACH ENERGY LEVEL
C      NS=33, PRINT ENERGY LEVELS ONLY
C      NS=OTHERWISE, DONT PRINT
       IF(NI-1)6,4,6
   4   EPRIN = E0*FACM
       WRITEOUTPUTTAPE6,5,KV,EPRIN
   5   FORMAT (47H1SCHR- SOLUTION OF RADIAL SCHR. EQUATION FOR V= I3, 5X
      Z          7HETRIAL= 1PE15.7,  9H   (1/CM)   )
       WRITEOUTPUTTAPE6,3
   3   FORMAT(70H0 ITER          E               F(E)              DF(E)
      X       D(E)       )
   6   CALL EFMT(K)
       H = (RMAX-RMIN)/FLOATF(N-1)
       H2=H**2
   8   HV=H2/12.
       E=E0
       TEST = -1.
       DE=0.
C
C      START ITER LOOP
C
  12   DO 171 IT=1,MAXIT
C      .....START INWARD INTEGRATION
  30   P(N)=1.E-30
  32   GN=V(N)-E
  34   GI=V(N-1)-E
C      .....TEST IF E TOO HIGH
       IF(GI) 35, 36, 36
  35   WRITEOUTPUTTAPE6,899
 899   FORMAT(50H DIFFERENCE EQUATION SOLUTION TECHNIQUE FAILS          )
       SCHR = 2.
       GO TO 250
  36   P(N-1)=P(N)*EXPF(RMAX*SQRTF(GN)-(RMAX-H)*SQRTF(GI))
  38   Y=(1.-HV*GN)*P(N)
  40   Y(2)=(1.-HV*GI)*P(N-1)
C      .....INTEGRATE
       K=0
  44   M=N-2
  46   Y(3)=Y(2)+((Y(2)-Y)+H2*GI*P(M+1))
  48   GI=V(M)-E
  50   P(M)=Y(3)/(1.-HV*GI)
C      .....TEST FOR OVERFLOW
  52   IF(K)54,70,54
C      .....OVERFLOW
  54   K=0
       M1=M+1
       PM=P(M1)
  55   DO 56 J=M1,N
  56   P(J)=P(J)/PM
  58   Y=Y/PM
  60   Y(2)=Y(2)/PM
```

Table III. (Contd.)

```
 62   Y(3)=Y(3)/PM                                            SCHRV058
      GI= V(M+1) - E                                          SCHRV059
      GO TO 46                                                SCHRV060
C     .....TEST FOR CROSSING PT.                              SCHRV061
 70   IF(ABSF(P(M))-ABSF(P(M+1))    ) 90, 90, 72              SCHRV062
72    IF(M-2)      90,90,81                                   SCHRV063
 81   Y= Y(2)                                                 SCHRV064
 82   Y(2)=Y(3)                                               SCHRV065
 84   M=M-1                                                   SCHRV066
 86   GO TO 46                                                SCHRV067
C                                                             SCHRV068
 90   PM=P(M)                                                 SCHRV069
      MSAVE = M                                               SCHRV070
 92   YIN=Y(2)/PM                                             SCHRV071
 94   DO 96 J=M,N                                             SCHRV072
 96   P(J)=P(J)/PM                                            SCHRV073
C                                                             SCHRV074
C     .....START OUTWARD INTEGRATION                          SCHRV075
C                                                             SCHRV076
 100  P(1)=1.E-20                                             SCHRV077
 102  Y=0.                                                    SCHRV078
 104  GI=V-E                                                  SCHRV079
 106  Y(2)=(1.-HV*GI)*P                                       SCHRV080
      K = 0                                                   SCHRV081
 108  DO 132 I=2,M                                            SCHRV082
 110  Y(3)=Y(2)+((Y(2)-Y)+H2*GI*P(I-1))                       SCHRV083
 112  GI=V(I)=E                                               SCHRV084
 114  P(I)=Y(3)/(1.-HV*GI)                                    SCHRV085
C     .....TEST FOR OVERFLOW                                  SCHRV086
 116  IF(K)118,130,118                                        SCHRV087
 118  K=0                                                     SCHRV088
      I1=I-1                                                  SCHRV089
      PM=P(I1)                                                SCHRV090
      DO 120 J=1,I1                                           SCHRV091
 120  P(J)=P(J)/PM                                            SCHRV092
 122  Y=Y/PM                                                  SCHRV093
 124  Y(2)=Y(2)/PM                                            SCHRV094
 126  Y(3)=Y(3)/PM                                            SCHRV095
      GI=V(I1)-E                                              SCHRV096
      GO TO 110                                               SCHRV097
C                                                             SCHRV098
 130  Y=Y(2)                                                  SCHRV099
 132  Y(2)=Y(3)                                               SCHRV100
C                                                             SCHRV101
C     .....FINISHED OUTWARD INTEGRATION                       SCHRV102
 134  PM=P(M)                                                 SCHRV103
      IF(PM)135,149,135                                       SCHRV104
 135  YOUT=Y/PM                                               SCHRV105
 136  YM=Y(3)/PM                                              SCHRV106
 138  DO 140 J=1,M                                            SCHRV107
 140  P(J)=P(J)/PM                                            SCHRV108
C                                                             SCHRV109
C     .....CORRECTION                                         SCHRV110
C                                                             SCHRV111
 142  DF=0.                                                   SCHRV112
 144  DO 146 J=1,N                                            SCHRV113
 146  DF=DF-P(J)**2                                           SCHRV114
 148  F=(-YOUT-YIN+2.*YM)/H2+(V(M)-E)                         SCHRV115
```

Table III. (Contd.)

```
      DOLD=DE                                                           SCHRV116
      IF(K)149,150,149                                                  SCHRV117
  149 F=9.999999E+29                                                    SCHRV118
      DF=-F                                                             SCHRV119
      DE=ABSF(.0001*E)                                                  SCHRV120
      GO TO 152                                                         SCHRV121
  150 DE=-F/DF                                                          SCHRV122
  152 IF(NI-1)164,162,164                                               SCHRV123
  156 FORMAT( 1H0     I4, 2X,  1P4E16.7,5X,29H THE CROSSING PT. OCCURS ASCHRV124
     1T        I4)                                                      SCHRV125
  162 EPRIN  = E*FACM                                                   SCHRV126
      DEPRIN = DE*FACM                                                  SCHRV127
      WRITEOUTPUTTAPE6,156,IT,EPRIN,F,DF,DEPRIN,MSAVE                   SCHRV128
  164 EOLD = E                                                          SCHRV129
      E=E+DE                                                            SCHRV130
  166 TEST=MAX1F(ABSF(DOLD)-ABSF(DE),TEST)                              SCHRV131
  168 IF(TEST)171,170,170                                               SCHRV132
  170 IF( ABSF( E-EOLD) - ABSF(EPS))  172,172,171                       SCHRV133
  171 CONTINUE                                                          SCHRV134
      SCHR=1.                                                           SCHRV135
      GO TO 173                                                         SCHRV136
C     .....CONVERGED-COUNT NODES                                        SCHRV137
  172 SCHR=0.                                                           SCHRV138
  173 KV=0                                                              SCHRV139
      NL=N-2                                                            SCHRV140
  174 DO 192 J=3,NL                                                     SCHRV141
  176 IF(P(J))178,177,177                                               SCHRV142
  177 IF(P(J-1))180,192,192                                             SCHRV143
  178 IF(P(J-1))192,270,184                                             SCHRV144
C     POS. NODE                                                         SCHRV145
  180 IF(P(J+1))192,182,182                                             SCHRV146
  182 IF(P(J-2))190,192,192                                             SCHRV147
C     NEG. NODE                                                         SCHRV148
  184 IF(P(J+1))186,192,192                                             SCHRV149
  186 IF(P(J-2))192,190,190                                             SCHRV150
C     FALSE NODE DUE TO UNDERFLOW                                       SCHRV151
  270 IF(P(J+1))280,192,192                                             SCHRV152
  280 IF(P(J-2))192,192,190                                             SCHRV153
  190 KV=KV+1                                                           SCHRV154
  192 CONTINUE                                                          SCHRV155
C     .....NORMALIZE                                                    SCHRV156
  200 SN=SQRTF(-H*DF)                                                   SCHRV157
  202 DO 204 J=1,N                                                      SCHRV158
  204 S(J)=P(J)/SN                                                      SCHRV159
C     .....PRINT SOLUTION                                               SCHRV160
  208 E = E*FACM                                                        SCHRV161
      IF(NS-1)236,210,236                                               SCHRV162
  210 IPSIA = IPSIQ * 300                                               SCHRV163
      IPSIB = IPSIQ *  49                                               SCHRV164
      IPSIC = IPSIQ * 250                                               SCHRV165
      IPSID = IPSIQ *  50                                               SCHRV166
      DO 234 JF=1,N,IPSIA                                               SCHRV167
  214 FORMAT(47H1SCHR- SOLUTION OF RADIAL SCHR. EQUATION FOR V= I3, 7H  SCHRV168
     X   E= 1PE15.7 /20H0   I        S(I)     5(20H     I        S(I)     ))SCHRV169
  218 WRITEOUTPUTTAPE6,214,KV,E                                         SCHRV170
  220 JL=XMINOF(JF+IPSIB,N)                                             SCHRV171
  222 DO 234 J=JF,JL,IPSIQ                                              SCHRV172
  224 IL=XMINOF(J+IPSIC,N)                                              SCHRV173
```

Table III. (Contd.)

```
 228   FORMAT(6(I5,1PE15.7))                                            SCHRV174
 232   WRITEOUTPUTTAPE6,228,(I,S(I),I=J,IL,IPSID)                       SCHRV175
 234   CONTINUE                                                         SCHRV176
 236   E0=E                                                             SCHRV177
       IF(NS-33) 874,875,874                                            SCHRV178
 875   WRITEOUTPUTTAPE6,876,KV,E                                        SCHRV179
876    FORMAT(50H0 SOLUTION OF RADIAL SCHRODINGER EQUATION FOR V = I3,  SCHRV180
      1 7H    E =  1PE15.7 )                                            SCHRV181
874    CONTINUE                                                         SCHRV182
 250   RETURN                                                           SCHRV183
       FREQUENCY 52(0,1,0),70(0,0,1),72(0,0,1),94(100),55(50),108(100),11SCHRV184
      16(0,1,0),138(100),144(200),152(1,0,0),           202(200)        SCHRV185
       END                                                              SCHRV186
```

Table III. (Contd.)

```
       COUNT    80
       LBL      EFMT
       REM NU EFM,EFM AND LFM FOR FORTRAN 2
       REM
       ENTRY EFM
       ENTRY EFMT
LFM    OCT 476000000004
       TTR 1,4
EFMT   CLA 1,4
       STA SETN+1
       CLA TTR
       TXI EFM+1,4,-1
EFM    CLA HPR
       STO OVER+2
       OCT 476000000002
SET    CLA X                       TTR  ANALY
       STO 8
       TTR 1,4
X      TTR ANALY
ANALY  SXD SAVEX,1
       LXD 0,1
       TTR *+14,1
       TTR MQO                   MQ OVER
SAVEX  PZE                         SAVE  XA IN DEC.,THEN  ACC.
       TTR ACMQ                    11
       TTR AC                       10
       TTR MQ                       9
ZERO   PZE
       TTR ACMQO                 AC AND MQ OVER
       TTR ACO
AC     CLA ZERO
       TTR RETRN
ACMQ   CLA ZERO                    3
       TTR MQ
MQ     LDQ ZERO                    1, MQ UNDER
RETRN  LXD SAVEX,1
       STO SAVEX
       CLA 0
       STA *+2
       CLA SAVEX
       TTR **
ACMQO  ORA MAX
MQO    STO SAVEA
       LLS 0
       LDQ MAX
       LRS 0
       TTR OVER+1
ACO    ORA MAX
OVER   STO SAVEA
       CLA 0
       HPR 63                    PAUSE OVERFLOW
       CLA SAVEA                 PRESS START TO CONTINUE
       TTR RETRN
SAVEA  PZE
THREE  PZE 0,0,3
TTR    TTR SETN
HPR    HPR 63
SETN   ANA THREE
       STO -
       TTR OVER+3
MAX    OCT 377777777777
       END
```

Table IV. Sample data deck for relative-intensity program.

```
*      DATA
1
1 SILICON NITRIDE INTENSITY DISTRIBUTION         TEST PROGRAM
   2  9.33526
   2   2  25     (2F10.0)
 1.3613170 12376.760
 1.3686189 11369.400
 1.3764643 10348.920
 1.3849046  9315.320
 1.3941121  8268.600
 1.4041987  7208.760
 1.4154399  6135.800
 1.4281304  5049.720
 1.4428560  3950.520
 1.4605683  2838.200
 1.4834289  1712.760
 1.5188710   574.200
 1.5718000      0.
 1.6311431   574.200
 1.6788244  1712.760
 1.7140474  2838.200
 1.7442476  3950.520
 1.7715936  5049.720
 1.7970281  6135.800
 1.8211572  7208.760
 1.8442578  8268.600
 1.8666328  9315.320
 1.8883695 10348.920
 1.9096753 11369.400
 1.9305798 12376.760
   1 50488.0
1.100      2.100      0.001        2
  10    2    1     (8XI2,F10.0)
            0   574.200
            1  1712.760
            2  2838.200
            3  3950.520
            4  5049.720
            5  6135.800
            6  7208.760
            7  8268.600
            8  9315.320
            9 10348.920
   2   2  25     (2F10.0)
 1.3841050 10068.404
 1.3882994  9287.577
 1.3935768  8499.421
 1.3999376  7699.832
 1.4074129  6885.047
 1.4160805  6051.643
 1.4261043  5196.535
 1.4377249  4316.981
 1.4514711  3410.577
 1.4682963  2475.260
 1.4903674  1509.307
 1.5254273   511.333
 1.5800000      0.
 1.6445856   511.333
```

Table IV. (Contd.)

```
 1.6996278  1509.307
 1.7421381  2475.260
 1.7798702  3410.577
 1.8149804  4316.981
 1.8404052  5196.535
 1.8806691  6051.643
 1.9119547  6885.047
 1.9423804  7699.832
 1.9719579  8499.421
 2.0006375  9287.577
 2.0283271 10068.404
   1 15872.0
1.100      2.100      0.001          2
   4   2   1    (8XI2,F10.0)
             0   511.333
             1  1509.307
             2  2475.260
             3  3410.577
   6   6  10  10 0.001


0.7310
0.00567

0.7235
0.01037

24300.0
  5
```

APPENDIX: COMPUTER OUTPUT OF SAMPLE DATA DECKS

Table V shows the computer output when the sample data deck given in Table II is run with the RKR program compiled from Table I; Table VI shows the computer output when the sample data deck given in Table IV is run with the relative-intensity program compiled from Table III.

Table V. RKR program output.

```
RKR PROCEDURE APPLIED TO THE X STATE OF SILICON NITRIDE   TEST PROGRAM
MOLECULAR CONSTANTS ARE TAKEN FROM JENKINS AND DE LASZLO


THE REDUCED MASS OF THE TWO ATOMS, BASED ON O16=16, IS   9.335260


TURNING POINTS ARE GENERATED BY CONSTANTS

THE G(V) CURVE IS CONSTRUCTED FROM THE FOLLOWING INPUT DATA.

WE =   1151.680, WEXE =    6.5600, WEYE =.          , WEZE =.          , WETE =.
TURNING POINTS ARE GENERATED BY CONSTANTS

THE BV(V) CURVE IS CONSTRUCTED FROM THE FOLLOWING INPUT DATA.

BE = 7.31000E-01, ALPHAE = 5.6700E-03, GAMMAE =-0.        , DELTAE =-0.        , EPSLNE =-0.
```

```
RKR PROCEDURE APPLIED TO THE X STATE OF SILICON NITRIDE   TEST PROGRAM
MOLECULAR CONSTANTS ARE TAKEN FROM JENKINS AND DE LASZLO

NUSBC IN BESRKR =  8.

THE G(V) VALUES USED BELOW ARE
```

V	G	V	G	V	G	V	G	V	G	V	G
0.	0.	0.500	574.2000	1.500	1712.7599	2.500	2838.1999	3.500	3950.5199	4.500	5049.7198
5.500	6135.7599	6.500	7208.7599	7.500	8268.5997	8.500	9315.3197	9.500	10348.3197		

```
THE BV(V) VALUES USED BELOW ARE
```

V	BV	V	BV	V	BV	V	BV	V	BV	V	BV
0.	0.7310000	0.500	0.7281650	1.500	0.7224950	2.500	0.7168250	3.500	0.7111550	4.500	0.7054850
5.500	0.6998150	6.500	0.6941450	7.500	0.5884750	8.500	0.6828050	9.500	0.6771350		

```
OUTPUT V,G--LEVELS AT WHICH TURNING POINTS ARE FOUND
```

V	G	V	G	V	G	V	G	V	G	V	G
0.500	574.2000	1.500	1712.7600	2.500	2838.2000	3.500	3950.5199	4.500	5049.7199	5.500	6135.7999
6.500	7208.7599	7.500	8268.5999	8.500	9315.3198	9.500	10348.9198				

Table V. (Contd.)

```
FOR V =   0.500, G =   574.200 1/CM, RMIN =  1.5188710 AND RMAX =  1.6311431 ANGSTROMS.  THIS REQUIRED  0.     SECONDS.
                 ALSO, BV =    0.7281650
                 THE KLEIN ACTION INTEGRALS F AND G ARE EQUAL TO  0.56136035E-01 0.22658374E-01

FOR V =   1.500, G =  1712.760 1/CM, RMIN =  1.4834289 AND RMAX =  1.6788244 ANGSTROMS.  THIS REQUIRED  0.     SECONDS.
                 ALSO, BV =    0.7224950
                 THE KLEIN ACTION INTEGRALS F AND G ARE EQUAL TO  0.97697736E-01 0.39229474E-01

FOR V =   2.500, G =  2838.200 1/CM, RMIN =  1.4605683 AND RMAX =  1.7140474 ANGSTROMS.  THIS REQUIRED  0.     SECONDS.
                 ALSO, BV =    0.7168250
                 THE KLEIN ACTION INTEGRALS F AND G ARE EQUAL TO  0.12673954E-00 0.50625280E-01

FOR V =   3.500, G =  3950.520 1/CM, RMIN =  1.4428560 AND RMAX =  1.7442476 ANGSTROMS.  THIS REQUIRED  0.     SECONDS.
                 ALSO, BV =    0.7111550
                 THE KLEIN ACTION INTEGRALS F AND G ARE EQUAL TO  0.15069580E-00 0.59878376E-01

FOR V =   4.500, G =  5049.720 1/CM, RMIN =  1.4281304 AND RMAX =  1.7715936 ANGSTROMS.  THIS REQUIRED  0.     SECONDS.
                 ALSO, BV =    0.7054850
                 THE KLEIN ACTION INTEGRALS F AND G ARE EQUAL TO  0.17173158E-00 0.67876304E-01

FOR V =   5.500, G =  6135.800 1/CM, RMIN =  1.4154399 AND RMAX =  1.7970281 ANGSTROMS.  THIS REQUIRED  0.     SECONDS.
                 ALSO, BV =    0.6998150
                 THE KLEIN ACTION INTEGRALS F AND G ARE EQUAL TO  0.19079412E-00 0.75009913E-01

FOR V =   6.500, G =  7208.760 1/CM, RMIN =  1.4041987 AND RMAX =  1.8211572 ANGSTROMS.  THIS REQUIRED  0.     SECONDS.
                 ALSO, BV =    0.6941450
                 THE KLEIN ACTION INTEGRALS F AND G ARE EQUAL TO  0.20847923E-00 0.81524249E-01

FOR V =   7.500, G =  8268.600 1/CM, RMIN =  1.3941121 AND RMAX =  1.8442578 ANGSTROMS.  THIS REQUIRED  0.     SECONDS.
                 ALSO, BV =    0.6884750
                 THE KLEIN ACTION INTEGRALS F AND G ARE EQUAL TO  0.22507283E-00 0.87539440E-01

FOR V =   8.500, G =  9315.320 1/CM, RMIN =  1.3849045 AND RMAX =  1.8666328 ANGSTROMS.  THIS REQUIRED  0.     SECONDS.
                 ALSO, BV =    0.6828050
                 THE KLEIN ACTION INTEGRALS F AND G ARE EQUAL TO  0.24086412E-00 0.93173706E-01

FOR V =   9.500, G = 10348.920 1/CM, RMIN =  1.3764643 AND RMAX =  1.8883695 ANGSTROMS.  THIS REQUIRED  0.     SECONDS.
                 ALSO, BV =    0.6771350
                 THE KLEIN ACTION INTEGRALS F AND G ARE EQUAL TO  0.25595257E-00 0.98470822E-01
```

Table VI. Relative-intensity program output.

SILICON NITRIDE INTENSITY DISTRIBUTION   TEST PROGRAM

THE REDUCED MASS OF THE TWO ATOMS, BASED ON O16=16, IS   9.335260

THE INPUT POTENTIAL POINTS, R IN ANGST. AND ENERGY IN 1/CM , ARE GIVEN BELOW.

R	V	R	V	R	V	R	V	R	V
1.361317	12376.7599	1.368619	11369.3999	1.376464	10348.9199	1.384905	9315.3199	1.394112	8268.6000
1.404199	7208.7599	1.415440	6135.8000	1.428130	5049.7200	1.442856	3950.5200	1.460568	2838.2000
1.483429	1712.7600	1.513871	574.2000	1.571800	0.	1.631143	574.2000	1.678824	1712.7600
1.714067	2838.2000	1.744248	3950.5200	1.771594	5049.7200	1.797028	6135.8000	1.821157	7208.7599
1.844258	8268.6000	1.866633	9315.3199	1.888369	10348.9199	1.909675	11369.3999	1.930530	12376.7599

DISSOCIATION ENERGY IN SAME UNITS AS ABOVE IS   0.50488000E 05

RMIN = 1.1000000, RMAX = 2.1000000, SPACING = 0.0010000, ALL IN ANGST.

THE TRIAL ENERGY LEVELS IN 1/CM ARE GIVEN BELOW.

LEVEL	ENERGY	LEVEL	ENERGY	LEVEL	ENERGY	LEVEL	ENERGY	LEVEL	ENERGY
0	5.7419999E 02	1	1.7127600E 03	2	2.8382000E 03	3	3.9505200E 03	4	5.0497200E 03
5	6.1358000E 03	6	7.2087600E 03	7	8.2686000E 03	8	9.3153199E 03	9	1.0348920E 04

THE INPUT POTENTIAL POINTS, R IN ANGST. AND ENERGY IN 1/CM , ARE GIVEN BELOW.

R	V	R	V	R	V	R	V	R	V
1.384105	10068.4039	1.388299	9287.5769	1.393577	8499.4209	1.399938	7699.8320	1.407413	6885.0470
1.416090	6051.6429	1.426104	5196.5350	1.437725	4316.9810	1.451471	3410.5770	1.468296	2475.2600
1.490367	1509.3070	1.525427	511.3330	1.580000	0.	1.644586	511.3330	1.699628	1509.3070
1.742138	2475.2600	1.779870	3410.5770	1.814980	4316.9810	1.848405	5196.5350	1.880569	6051.6429
1.911955	6885.0470	1.942380	7699.8320	1.971958	8499.4209	2.000637	9287.5769	2.028327	10068.4039

DISSOCIATION ENERGY IN SAME UNITS AS ABOVE IS   0.15871999E 05

RMIN = 1.1000000, RMAX = 2.1000000, SPACING = 0.0010000, ALL IN ANGST.

THE TRIAL ENERGY LEVELS IN 1/CM ARE GIVEN BELOW.

LEVEL	ENERGY	LEVEL	ENERGY	LEVEL	ENERGY	LEVEL	ENERGY	LEVEL	ENERGY
0	5.1133299E 02	1	1.5093070E 03	2	2.4752600E 03	3	3.4105770E 03		

CONVERGENCE CRITERION IS ERROR LESS THAN 1.00E-03 1/CM

Table VI. (Contd.)

SILICON NITRIDE INTENSITY DISTRIBUTION . TEST PROGRAM

TIME BEFORE POTFIT = 0.

LEFT END OF POTENTIAL FUNCTION IS FOUND FROM Y=A/X**12+C, WHERE A = 6.5624240E 05 AND C = -5.4312680E 04

RIGHT END OF POTENTIAL FUNCTION IS FOUND FROM Y=A/X**B, WHERE A = -0.1843505E 06 AND B = 0.2396292E 01

TIME FOR POTFIT = 0.

THE POTENTIAL FUNCTION GENERATED IS

R(A)	V(1/CM)	R(A)	V(1/CM)	R(A)	V(1/CM)	R(A)	V(1/CM)	R(A)	V(1/CM)	
1.100000	205274.6602	1.105000	194199.1992	1.110000	183756.4551	1.115000	173907.6738	1.120000	164616.6484	21
1.125000	155849.4902	1.130000	147574.5371	1.135000	139762.1484	1.140000	132384.6191	1.145000	125415.9453	46
1.150000	118831.8906	1.155000	112609.6572	1.160000	106727.9414	1.165000	101166.7441	1.170000	95907.3340	71
1.175000	90932.1533	1.180000	86224.7275	1.185000	81769.5977	1.190000	77552.2588	1.195000	73559.1143	96
1.200000	69777.3779	1.205000	66195.0381	1.210000	62800.8188	1.215000	59584.1284	1.220000	56535.0068	121
1.225000	53644.0840	1.230000	50902.5591	1.235000	48302.1587	1.240000	45835.0869	1.245000	43494.0078	146
1.250000	41272.0205	1.255000	39162.6240	1.260000	37159.6997	1.265000	35257.4858	1.270000	33450.5459	171
1.275000	31733.7578	1.280000	30102.3035	1.285000	28551.6296	1.290000	27077.4470	1.295000	25675.7041	196
1.300000	24342.5852	1.305000	23074.4841	1.310000	21867.9983	1.315000	20719.9128	1.320000	19627.2021	221
1.325000	18586.9966	1.330000	17596.5886	1.335000	16653.4219	1.340000	15755.0769	1.345000	14899.2701	246
1.350000	14083.8391	1.355000	13306.7396	1.360000	12566.0364	1.365000	11859.6443	1.370000	11185.7922	271
1.375000	10535.2366	1.380000	9907.3490	1.385000	9304.0481	1.390000	8725.9846	1.395000	8171.7239	296
1.400000	7639.0359	1.405000	7128.5466	1.410000	6641.1568	1.415000	6175.7377	1.420000	5730.6632	321
1.425000	5305.6486	1.430000	4900.7443	1.435000	4515.9811	1.440000	4150.6864	1.445000	3804.0929	345
1.450000	3475.4547	1.455000	3164.4078	1.460000	2870.5324	1.465000	2593.6631	1.470000	2333.3247	371
1.475000	2089.1022	1.480000	1860.5940	1.485000	1647.3567	1.490000	1448.9069	1.495000	1264.9209	396
1.500000	1095.0128	1.505000	938.8093	1.510000	795.9440	1.515000	666.0608	1.520000	548.8205	421
1.525000	443.9079	1.530000	350.9660	1.535000	269.6675	1.540000	199.6944	1.545000	140.7352	446
1.550000	92.4844	1.555000	54.6443	1.560000	26.9235	1.565000	9.0385	1.570000	0.7111	471
1.575000	1.6714	1.580000	11.6533	1.585000	30.3970	1.590000	57.6488	1.595000	93.1608	496
1.600000	136.6916	1.605000	188.0049	1.610000	246.8704	1.615000	313.0620	1.620000	386.3606	521
1.625000	466.5507	1.630000	553.4224	1.635000	646.7746	1.640000	746.4041	1.645000	852.1140	546
1.650000	963.7133	1.655000	1081.0151	1.660000	1203.8379	1.665000	1332.0043	1.670000	1465.3398	571
1.675000	1603.6760	1.680000	1746.8437	1.685000	1894.6728	1.690000	2047.0255	1.695000	2203.7491	596
1.700000	2364.6935	1.705000	2529.7126	1.710000	2698.6600	1.715000	2871.4026	1.720000	3047.8218	621
1.725000	3227.7375	1.730000	3411.0101	1.735000	3597.5085	1.740000	3787.1060	1.745000	3979.6739	646
1.750000	4175.0609	1.755000	4373.2339	1.760000	4574.1024	1.765000	4777.5763	1.770000	4983.5575	671
1.775000	5192.0093	1.780000	5402.7653	1.785000	5615.6592	1.790000	5830.5624	1.795000	6047.3519	696
1.800000	6265.8502	1.805000	6486.0188	1.810000	6707.8674	1.815000	6931.3579	1.820000	7156.4438	721
1.825000	7383.1766	1.830000	7611.3573	1.835000	7840.8148	1.840000	8071.4157	1.845000	8303.0166	746
1.850000	8535.4229	1.855000	8768.7688	1.860000	9003.0602	1.865000	9238.2977	1.870000	9474.4625	771
1.875000	9711.5092	1.880000	9949.3544	1.885000	10187.8752	1.890000	10426.9159	1.895000	10666.2990	796
1.900000	10905.8463	1.905000	11145.4172	1.910000	11385.3303	1.915000	11629.5367	1.920000	11871.5869	821
1.925000	12111.5048	1.930000	12349.3149	1.935000	12585.0442	1.940000	12818.7108	1.945000	13050.3424	846
1.950000	13279.9598	1.955000	13507.5880	1.960000	13733.2465	1.965000	13956.9574	1.970000	14178.7441	871
1.975000	14398.6281	1.980000	14616.6288	1.985000	14832.7671	1.990000	15047.0646	1.995000	15259.5416	896
2.000000	15470.2192	2.005000	15679.1121	2.010000	15886.2465	2.015000	16091.6366	2.020000	16295.3030	921
2.025000	16497.2644	2.030000	16697.5393	2.035000	16896.1458	2.040000	17093.1035	2.045000	17288.4270	946
2.050000	17482.1350	2.055000	17674.2454	2.060000	17864.7749	2.065000	18053.7412	2.070000	18241.1592	971
2.075000	18427.0457	2.080000	18611.4172	2.085000	18794.2893	2.090000	18975.6775	2.095000	19155.5991	996

TIME FOR PRINT OF POTENTIAL = 0. SECONDS.

Table VI. (Contd.)

SILICON NITRIDE INTENSITY DISTRIBUTION TEST PROGRAM

LEFT END OF POTENTIAL FUNCTION IS FOUND FROM Y=A/X**12+C, WHERE A = 1.0824779E 06 AND C = -2.7700926E 04

RIGHT END OF POTENTIAL FUNCTION IS FOUND FROM Y=A/X**B, WHERE A = -0.3839180E 07 AND B = 0.9183305E 01

TIME FOR POTFIT = 0.

THE POTENTIAL FUNCTION GENERATED IS

R(A)	V(1/CM)	R(A)	V(1/CM)	R(A)	V(1/CM)	R(A)	V(1/CM)	R(A)	V(1/CM)	
1.100000	333082.3633	1.105000	314813.2891	1.110000	297587.8828	1.115000	281342.2344	1.120000	266016.6016	21
1.125000	251555.0938	1.130000	237905.4756	1.135000	225018.8730	1.140000	212849.5664	1.145000	201354.6758	46
1.150000	190494.2188	1.155000	180230.5879	1.160000	170528.6445	1.165000	161355.3965	1.170000	152679.9531	71
1.175000	144473.3438	1.180000	136708.4023	1.185000	129359.6260	1.190000	122403.0869	1.195000	115816.3584	96
1.200000	109578.3477	1.205000	103669.2451	1.210000	98070.4512	1.215000	92764.4902	1.220000	87734.9346	121
1.225000	82966.3320	1.230000	78444.1611	1.235000	74154.7754	1.240000	70085.3184	1.245000	66223.6875	146
1.250000	62558.4990	1.255000	59079.0308	1.260000	55775.1885	1.265000	52637.4688	1.270000	49655.9048	171
1.275000	46825.0479	1.280000	44133.9478	1.285000	41576.0977	1.290000	39144.4199	1.295000	36832.2319	196
1.300000	34633.2397	1.305000	32541.4956	1.310000	30551.3860	1.315000	28657.6079	1.320000	26855.1719	221
1.325000	25139.3435	1.330000	23505.6565	1.335000	21949.8940	1.340000	20468.0662	1.345000	19055.4048	246
1.350000	17711.3440	1.355000	16429.5110	1.360000	15207.7144	1.365000	14042.9445	1.370000	12932.3400	271
1.375000	11873.1987	1.380000	10862.9611	1.385000	9884.9602	1.390000	9016.0759	1.395000	8309.4109	296
1.400000	7692.5469	1.405000	7136.3415	1.410000	6625.4777	1.415000	6150.2122	1.420000	5705.0557	321
1.425000	5285.9261	1.430000	4889.3934	1.435000	4513.5172	1.440000	4157.3465	1.445000	3820.1700	345
1.450000	3501.1172	1.455000	3199.1960	1.460000	2913.7604	1.465000	2644.3413	1.470000	2390.4904	371
1.475000	2151.8147	1.480000	1927.9307	1.485000	1718.4811	1.490000	1523.1176	1.495000	1341.4402	396
1.500000	1173.1340	1.505000	1017.8584	1.510000	875.2619	1.515000	744.9872	1.520000	626.6684	421
1.525000	519.9307	1.530000	424.1486	1.535000	339.1136	1.540000	264.4832	1.545000	199.8984	446
1.550000	145.0051	1.555000	99.4539	1.560000	62.9005	1.565000	35.0074	1.570000	15.4422	471
1.575000	3.8795	1.580000	-0.	1.585000	3.4838	1.590000	14.0345	1.595000	31.3561	496
1.600000	55.1595	1.605000	85.1637	1.610000	121.0958	1.615000	162.6905	1.620000	209.6907	521
1.625000	261.8468	1.630000	318.9180	1.635000	380.6708	1.640000	446.8793	1.645000	517.3263	546
1.650000	591.7890	1.655000	670.0799	1.660000	752.0042	1.665000	837.3752	1.670000	926.0130	571
1.675000	1017.7440	1.680000	1112.4018	1.685000	1209.8268	1.690000	1309.8631	1.695000	1412.3639	596
1.700000	1517.1881	1.705000	1624.2155	1.710000	1733.2920	1.715000	1844.2899	1.720000	1957.0878	621
1.725000	2071.5687	1.730000	2187.6226	1.735000	2305.1423	1.740000	2424.0285	1.745000	2544.1825	645
1.750000	2665.5164	1.755000	2787.9460	1.760000	2911.3916	1.765000	3035.7765	1.770000	3161.0305	671
1.775000	3287.0844	1.780000	3413.3755	1.785000	3541.3351	1.790000	3669.4180	1.795000	3798.0745	696
1.800000	3927.2545	1.805000	4056.9131	1.810000	4187.0065	1.815000	4317.4925	1.820000	4448.3563	721
1.825000	4579.5283	1.830000	4710.9673	1.835000	4842.6364	1.840000	4974.5015	1.845000	5106.5333	746
1.850000	5238.6945	1.855000	5370.9554	1.860000	5503.3289	1.865000	5635.8083	1.870000	5768.3916	771
1.875000	5901.0767	1.880000	6033.3647	1.885000	6166.7785	1.890000	6299.7972	1.895000	6432.9152	796
1.900000	6566.1324	1.905000	6699.4464	1.910000	6832.8605	1.915000	6966.3719	1.920000	7099.9904	821
1.925000	7233.7340	1.930000	7367.5164	1.935000	7501.6541	1.940000	7635.3669	1.945000	7770.2760	846
1.950000	7904.9041	1.955000	8039.7776	1.960000	8174.9232	1.965000	8310.3715	1.970000	8446.1519	871
1.975000	8582.2997	1.980000	8718.3488	1.985000	8855.8389	1.990000	8993.3083	1.995000	9131.3016	896
2.000000	9269.8649	2.005000	9417.9734	2.010000	9563.9174	2.015000	9706.2119	2.020000	9844.9547	921
2.025000	9980.2441	2.030000	10112.1746	2.035000	10240.8367	2.040000	10366.3202	2.045000	10488.7103	946
2.050000	10608.0906	2.055000	10724.5422	2.060000	10838.1436	2.065000	10948.9719	2.070000	11057.1008	971
2.075000	11162.6027	2.080000	11265.5474	2.085000	11366.0016	2.090000	11464.0341	2.095000	11559.7064	996

TIME FOR PRINT OF POTENTIAL = 0. SECONDS.

SCHR FINDS ENERGY LEVEL G = 510.74768 1/CM AND BV = 0.7183588 1/CM IN 0. SECONDS.

SCHR FINDS ENERGY LEVEL G = 1508.87561 1/CM AND BV = 0.7079762 1/CM IN 0. SECONDS.

SCHR FINDS ENERGY LEVEL G = 2475.04663 1/CM AND BV = 0.6975725 1/CM IN 0. SECONDS.

Table VI. (Contd.)

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SCHR FINDS ENERGY LEVEL G =  3410.83838 1/CM AND BV =   0.6871293 1/CM IN  0.    SECONDS.
SCHR FINDS ENERGY LEVEL G =   574.28906 1/CM AND BV =   0.7281663 1/CM IN  0.    SECONDS.
SCHR FINDS ENERGY LEVEL G =  1712.95313 1/CM AND BV =   0.7224968 1/CM IN  0.    SECONDS.
SCHR FINDS ENERGY LEVEL G =  2838.48242 1/CM AND BV =   0.7168278 1/CM IN  0.    SECONDS.
SCHR FINDS ENERGY LEVEL G =  3950.87549 1/CM AND BV =   0.7111584 1/CM IN  0.    SECONDS.
SCHR FINDS ENERGY LEVEL G =  5050.12109 1/CM AND BV =   0.7054850 1/CM IN  0.    SECONDS.
SCHR FINDS ENERGY LEVEL G =  6136.20654 1/CM AND BV =   0.6998171 1/CM IN  0.    SECONDS.
SCHR FINDS ENERGY LEVEL G =  7209.21094 1/CM AND BV =   0.6941557 1/CM IN  0.    SECONDS.
SCHR FINDS ENERGY LEVEL G =  8269.12012 1/CM AND BV =   0.6884710 1/CM IN  0.    SECONDS.
SCHR FINDS ENERGY LEVEL G =  9315.89746 1/CM AND BV =   0.6827840 1/CM IN  0.    SECONDS.
SCHR FINDS ENERGY LEVEL G = 10349.67578 1/CM AND BV =   0.6770849 1/CM IN  0.    SECONDS.
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SILICON NITRIDE INTENSITY DISTRIBUTION TEST PROGRAM

PROGRAM SUCCESSFUL. (MAXIT REACHED 0 TIMES)

THE BELOW IS FOR THE LOWER STATE.

DIFFERENCE = CALC. - GIVEN

VIB. NO.	GIVEN ENERGY	CALC. ENERGY	DIFFERENCE	GIVEN DELTA G	CALC. DELTA G	DIFFERENCE
0	574.20011	574.28906	0.08895	1138.56004	1138.66406	0.10402
1	1712.76016	1712.95313	0.19296	1125.44006	1125.52930	0.08923
2	2838.20023	2838.48242	0.28220	1112.31970	1112.39307	0.07336
3	3950.51993	3950.87549	0.35556	1099.20010	1099.24561	0.04550
4	5049.72003	5050.12109	0.40106	1086.07971	1086.08545	0.00574
5	6135.79974	6136.20654	0.40680	1072.96014	1073.00439	0.04425
6	7208.75989	7209.21094	0.45105	1059.83972	1059.90918	0.06946
7	8268.59961	8269.12012	0.52051	1046.72021	1046.77734	0.05713
8	9315.31982	9315.89746	0.57764	1033.59985	1033.77832	0.17847
9	10348.91968	10349.67578	0.75610			

Table VI. (Contd.) UCRL-10925

VIB. NO.	CALC. BV
0	0.72816626
1	0.72249678
2	0.71682784
3	0.71115841
4	0.70548503
5	0.69981708
6	0.69415566
7	0.68847096
8	0.68278404
9	0.67708492

SILICON NITRIDE INTENSITY DISTRIBUTION TEST PROGRAM

THE BELOW IS FOR THE UPPER STATE.

VIB. NO.	GIVEN ENERGY	CALC. ENERGY	DIFFERENCE DIFFERENCE = CALC. - GIVEN
0	511.33312	510.74768	-0.58544
1	1509.30696	1508.87561	-0.43135
2	2475.26004	2475.04663	-0.21341
3	3410.57684	3410.83838	0.26154

VIB. NO.	CALC. BV
0	0.71835880
1	0.70797616
2	0.69757245
3	0.68712933

Table VI. (Contd.)

FRANCK-CONDON FACTORS

V''	V' = 0	V' = 1	V' = 2	V' = 3
0	0.9812E 00	0.1862E-01	0.9118E-04	0.4651E-04
1	0.1691E-01	0.9232E 00	0.5966E-01	0.2385E-07
2	0.1769E-02	0.5015E-01	0.8193E 00	0.1274E-00
3	0.8105E-04	0.7427E-02	0.9868E-01	0.6680E 00
4	0.4064E-05	0.5441E-03	0.1995E-01	0.1549E-00
5	0.1551E-06	0.3818E-04	0.2149E-02	0.4233E-01
6	0.1278E-07	0.2180E-05	0.2003E-03	0.6418E-02
7	0.3751E-09	0.1336E-06	0.1611E-04	0.7658E-03
8	0.1501E-09	0.1471E-07	0.8705E-06	0.8276E-04
9	0.4100E-09	0.3401E-08	0.1801E-06	0.4551E-05

R-CENTROID FACTORS (ANGSTROMS)

V''	V' = 0	V' = 1	V' = 2	V' = 3
0	0.1582E 01	0.1300E 01	0.2791E 01	0.1710E 01
1	0.1906E 01	0.1593E 01	0.1383E 01	0.1489E 03
2	0.1733E 01	0.1864E 01	0.1603E 01	0.1442E 01
3	0.1911E 01	0.1763E 01	0.1842E 01	0.1611E 01
4	0.1894E 01	0.1898E 01	0.1786E 01	0.1830E 01
5	0.2009E 01	0.1904E 01	0.1892E 01	0.1804E 01
6	0.1888E 01	0.1980E 01	0.1915E 01	0.1890E 01
7	0.2056E 01	0.1994E 01	0.1962E 01	0.1927E 01
8	0.1321E 01	0.1838E 01	0.2078E 01	0.1953E 01
9	0.1439E 01	0.1261E 01	0.1788E 01	0.2129E 01

R**2-CENTROIDS

V''	V' = 0	V' = 1	V' = 2	V' = 3
0	0.2503E 01	0.1611E 01	0.6121E 01	0.2761E 01
1	0.3532E 01	0.2542E 01	0.1872E 01	0.4512E 03
2	0.3044E 01	0.3406E 01	0.2579E 01	0.2059E 01
3	0.3587E 01	0.3137E 01	0.3341E 01	0.2609E 01
4	0.3615E 01	0.3560E 01	0.3209E 01	0.3311E 01
5	0.3977E 01	0.3640E 01	0.3550E 01	0.3268E 01
6	0.3616E 01	0.3890E 01	0.3673E 01	0.3552E 01
7	0.4176E 01	0.3977E 01	0.3838E 01	0.3711E 01
8	0.1626E 01	0.3451E 01	0.4265E 01	0.3812E 01
9	0.2080E 01	0.1449E 01	0.3291E 01	0.4440E 01

Table VI. (Contd.)

RELATIVE INTENSITY(QUANTUM/SEC) SCALED TO TEN

V''	V' = 0	V' = 1	V' = 2	V' = 3
0	10.000	0.232	0.001	0.001
1	0.149	10.000	0.836	0.000
2	0.013	0.471	10.000	2.188
3	0.001	0.060	1.044	10.000
4	0.000	0.004	0.182	2.011
5	0.000	0.000	0.017	0.474
6	0.000	0.000	0.001	0.052
7	0.000	0.000	0.000	0.006
8	0.000	0.000	0.000	0.001
9	0.000	0.000	0.000	0.000

RELATIVE INTENSITY(ENERGY/SEC) SCALED TO TEN

V''	V' = 0	V' = 1	V' = 2	V' = 3
0	10.000	0.243	0.002	0.001
1	0.142	10.000	0.875	0.000
2	0.012	0.449	10.000	2.291
3	0.000	0.054	0.996	10.000
4	0.000	0.003	0.165	1.918
5	0.000	0.000	0.014	0.431
6	0.000	0.000	0.001	0.053
7	0.000	0.000	0.000	0.005
8	0.000	0.000	0.000	0.000
9	0.000	0.000	0.000	0.000

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CONSTANTS
0
0
    0.24299999E 05
    0.73100000E 00
    0.72350000E 00
    0.56699999E-02
    0.10370000E-01
   -0.
   -0.

TIME =     0.
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REFERENCES

1. R. N. Zare, Lawrence Radiation Laboratory Report UCRL-11110, November 1963, J. Chem. Phys. (to be published).

2. All timing information refers to IBM 7094.

3. R. N. Zare and J. K. Cashion, Lawrence Radiation Laboratory Report UCRL-10881, July 1963 (unpublished).